

3,6,9,12-TETRAOXA-1-TETRACOSANOL

Other names:	3,6,9,12-Tetraoxa-1-tetracosanol 3,6,9,12-Tetraoxatetracosan-1-ol Ethanol, 2-(2-(2-(2-(dodecyloxy)ethoxy)ethoxy)ethoxy)- LA 4 Laureth-4 Lauryl alcohol tri(oxyethylene) ethanol Mulsifan CPA NSC 190605 Polyoxyethylene(4) lauryl ether Tetra(oxydiethanol) monodecyl ether Tetra(oxyethylene) dodecyl ether Tetraethylene glycol dodecyl ether Tetraethylene glycol mono-n-dodecyl ether Tetraethylene glycol monolauryl ether Tetraoxyethylene glycol monododecyl ether n-Dodecyl tetraethylene glycol ether
Inchi:	InChI=1S/C20H42O5/c1-2-3-4-5-6-7-8-9-10-11-13-22-15-17-24-19-20-25-18-16-23-14-12
InchiKey:	WPMWEXCIYCJSA-UHFFFAOYSA-N
Formula:	C20H42O5
SMILES:	CCCCCCCCCCCCOCCOCCOCCOCCO
Mol. weight [g/mol]:	362.55

Physical Properties

Property code	Value	Unit	Source
af	1.2560		Cheméo Relay (1.0)
gf	-439.30	kJ/mol	Joback Method
hf	-1107.38	kJ/mol	Cheméo Relay (1.0)
hfus	56.40	kJ/mol	Joback Method
hvap	119.64	kJ/mol	Cheméo Relay (1.0)
ie	9.83	eV	Cheméo Relay (1.0)
log10ws	-4.17		Cheméo Relay (1.0)
logp	3.966		Crippen Method
mcvol	322.010	ml/mol	McGowan Method
pc	1031.25	kPa	Joback Method
tb	659.60	K	Cheméo Relay (1.0)
tc	827.40	K	Cheméo Relay (1.0)
tf	282.88	K	Cheméo Relay (1.0)

vc	1.250	m3/kmol	Cheméo Relay (1.0)
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Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1142.38	J/mol×K	996.72	Joback Method
cpg	1155.68	J/mol×K	1028.29	Joback Method
cpg	1077.24	J/mol×K	870.43	Joback Method
cpg	1095.33	J/mol×K	902.00	Joback Method
cpg	1112.21	J/mol×K	933.57	Joback Method
cpg	1127.89	J/mol×K	965.15	Joback Method
cpg	1057.95	J/mol×K	838.86	Joback Method
dvisc	0.0000480	Pa×s	589.55	Joback Method
dvisc	0.0001161	Pa×s	527.23	Joback Method
dvisc	0.0003555	Pa×s	464.90	Joback Method
dvisc	0.0000235	Pa×s	651.88	Joback Method
dvisc	0.0000130	Pa×s	714.21	Joback Method
dvisc	0.0000080	Pa×s	776.53	Joback Method
dvisc	0.0000052	Pa×s	838.86	Joback Method
hvapt	135.50	kJ/mol	522.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5274680&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity

dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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