

hexadecyl docosanoate

Other names:	hexadecyl docosanoate
Inchi:	InChI=1S/C38H76O2/c1-3-5-7-9-11-13-15-17-19-20-21-22-23-24-26-28-30-32-34-36-38
InchiKey:	UEDYHQHDUXDFGA-UHFFFAOYSA-N
Formula:	C38H76O2
SMILES:	CCCCCCCCCCCCCCCCCCCCCCCC(=O)OCCCCCCCCCCCCCCCC
Mol. weight [g/mol]:	565.01
CAS:	42233-11-4

Physical Properties

Property code	Value	Unit	Source
gf	35.16	kJ/mol	Joback Method
hf	-1072.45	kJ/mol	Joback Method
hfus	96.96	kJ/mol	Joback Method
hvap	109.34	kJ/mol	Joback Method
log10ws	-14.59		Crippen Method
logp	13.833		Crippen Method
mcvol	553.720	ml/mol	McGowan Method
pc	430.43	kPa	Joback Method
rinpol	3946.89		NIST Webbook
rinpol	3946.89		NIST Webbook
tb	1145.13	K	Joback Method
tc	1530.59	K	Joback Method
tf	291.50 ± 0.70	K	NIST Webbook
vc	2.188	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2091.96	J/molxK	1145.13	Joback Method
cpg	2240.98	J/molxK	1466.35	Joback Method
cpg	2217.78	J/molxK	1402.10	Joback Method
cpg	2191.88	J/molxK	1337.86	Joback Method
cpg	2162.67	J/molxK	1273.62	Joback Method
cpg	2129.57	J/molxK	1209.37	Joback Method

cpg	2262.08	J/molxK	1530.59	Joback Method
dvisc	0.0000046	Paxs	1145.13	Joback Method
dvisc	0.0000064	Paxs	1052.64	Joback Method
dvisc	0.0000094	Paxs	960.15	Joback Method
dvisc	0.0000151	Paxs	867.66	Joback Method
dvisc	0.0000272	Paxs	775.16	Joback Method
dvisc	0.0000572	Paxs	682.67	Joback Method
dvisc	0.0001520	Paxs	590.18	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C42233114&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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