

Heptaethylene glycol monododecyl ether

Other names:	3,6,9,12,15,18,21-Heptaoxatritriacontan-1-ol C ₁₂ H ₂₅ (OC ₂ H ₄) ₇ OH 3,6,9,12,15,18,21-heptaoxatritriacontanol
Inchi:	InChI=1S/C ₂₆ H ₅₄ O ₈ /c1-2-3-4-5-6-7-8-9-10-11-13-28-15-17-30-19-21-32-23-25-34-26-2
InchiKey:	DWHIUNMOTRUVPG-UHFFFAOYSA-N
Formula:	C ₂₆ H ₅₄ O ₈
SMILES:	CCCCCCCCCCCCOCCOCCOCCOCCOCCOCCOCCO
Mol. weight [g/mol]:	494.70
CAS:	3055-97-8

Physical Properties

Property code	Value	Unit	Source
gf	-703.78	kJ/mol	Joback Method
hf	-1657.74	kJ/mol	Joback Method
hfus	75.50	kJ/mol	Joback Method
hvap	107.02	kJ/mol	Joback Method
log10ws	-3.58		Crippen Method
logp	4.016		Crippen Method
mcvol	424.160	ml/mol	McGowan Method
pc	714.54	kPa	Joback Method
tb	1043.40	K	Joback Method
tc	1340.32	K	Joback Method
tf	599.21	K	Joback Method
vc	1.637	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1531.12	J/mol×K	1043.40	Joback Method
cpg	1593.49	J/mol×K	1290.84	Joback Method
cpg	1589.97	J/mol×K	1241.35	Joback Method
cpg	1581.92	J/mol×K	1191.86	Joback Method
cpg	1569.39	J/mol×K	1142.37	Joback Method
cpg	1552.44	J/mol×K	1092.89	Joback Method

cpg	1592.42	J/mol×K	1340.32	Joback Method
dvisc	0.0000006	Paxs	1043.40	Joback Method
dvisc	0.0000009	Paxs	969.37	Joback Method
dvisc	0.0000014	Paxs	895.34	Joback Method
dvisc	0.0000024	Paxs	821.31	Joback Method
dvisc	0.0000045	Paxs	747.27	Joback Method
dvisc	0.0000098	Paxs	673.24	Joback Method
dvisc	0.0000262	Paxs	599.21	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3055978&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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