

Diglycolic acid, heptadecyl neopentyl ester

Inchi:	InChI=1S/C26H50O5/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-30-24(27)21-29-2
InchiKey:	YJXFUGFTIMTRNR-UHFFFAOYSA-N
Formula:	C26H50O5
SMILES:	CCCCCCCCCCCCCCCCOC(=O)COCC(=O)OCC(C)(C)C
Mol. weight [g/mol]:	442.67

Physical Properties

Property code	Value	Unit	Source
gf	-401.96	kJ/mol	Joback Method
hf	-1210.54	kJ/mol	Joback Method
hfus	62.44	kJ/mol	Joback Method
hvap	92.90	kJ/mol	Joback Method
log10ws	-7.28		Crippen Method
logp	7.007		Crippen Method
mcvol	397.950	ml/mol	McGowan Method
pc	763.10	kPa	Joback Method
rinsol	3591.00		NIST Webbook
tb	966.05	K	Joback Method
tc	1189.08	K	Joback Method
tf	551.75	K	Joback Method
vc	1.546	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1376.87	J/molxK	966.05	Joback Method
cpg	1397.41	J/molxK	1003.22	Joback Method
cpg	1416.21	J/molxK	1040.39	Joback Method
cpg	1433.34	J/molxK	1077.56	Joback Method
cpg	1448.85	J/molxK	1114.73	Joback Method
cpg	1462.80	J/molxK	1151.91	Joback Method
cpg	1475.24	J/molxK	1189.08	Joback Method
dvisc	0.0002423	Paxs	551.75	Joback Method
dvisc	0.0001113	Paxs	620.80	Joback Method

dvisc	0.0000598	Paxs	689.85	Joback Method
dvisc	0.0000359	Paxs	758.90	Joback Method
dvisc	0.0000235	Paxs	827.95	Joback Method
dvisc	0.0000164	Paxs	897.00	Joback Method
dvisc	0.0000121	Paxs	966.05	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=U381928&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
mccvol:	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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