

Diglycolic acid, hexadecyl pentyl ester

Inchi:	InChI=1S/C25H48O5/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-19-21-30-25(27)23-28-22-2
InchiKey:	RXTJTPZXBPXAES-UHFFFAOYSA-N
Formula:	C25H48O5
SMILES:	CCCCCCCCCCCCCCCCOC(=O)COCC(=O)OCCCCC
Mol. weight [g/mol]:	428.65

Physical Properties

Property code	Value	Unit	Source
gf	-413.22	kJ/mol	Joback Method
hf	-1181.15	kJ/mol	Joback Method
hfus	67.27	kJ/mol	Joback Method
hvap	91.97	kJ/mol	Joback Method
log10ws	-7.10		Crippen Method
logp	6.761		Crippen Method
mcvol	383.860	ml/mol	McGowan Method
pc	796.63	kPa	Joback Method
rinpol	3740.00		NIST Webbook
rinpol	3740.00		NIST Webbook
tb	946.40	K	Joback Method
tc	1165.45	K	Joback Method
tf	538.06	K	Joback Method
vc	1.502	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1313.24	J/molxK	946.40	Joback Method
cpg	1398.15	J/molxK	1128.94	Joback Method
cpg	1384.56	J/molxK	1092.43	Joback Method
cpg	1369.31	J/molxK	1055.93	Joback Method
cpg	1352.36	J/molxK	1019.42	Joback Method
cpg	1333.68	J/molxK	982.91	Joback Method
cpg	1410.09	J/molxK	1165.45	Joback Method
dvisc	0.0000186	Paxs	946.40	Joback Method

dvisc	0.0000248	Paxs	878.34	Joback Method
dvisc	0.0000347	Paxs	810.29	Joback Method
dvisc	0.0000517	Paxs	742.23	Joback Method
dvisc	0.0000835	Paxs	674.17	Joback Method
dvisc	0.0001502	Paxs	606.12	Joback Method
dvisc	0.0003132	Paxs	538.06	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381854&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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