

Diglycolic acid, dodecyl neopentyl ester

Inchi:	InChI=1S/C21H40O5/c1-5-6-7-8-9-10-11-12-13-14-15-25-19(22)16-24-17-20(23)26-18-2
InchiKey:	VNCPMPLZWOGOLO-UHFFFAOYSA-N
Formula:	C21H40O5
SMILES:	CCCCCCCCCCCCOC(=O)COCC(=O)OCC(C)(C)C
Mol. weight [g/mol]:	372.54

Physical Properties

Property code	Value	Unit	Source
gf	-444.06	kJ/mol	Joback Method
hf	-1107.34	kJ/mol	Joback Method
hfus	49.49	kJ/mol	Joback Method
hvap	81.77	kJ/mol	Joback Method
log10ws	-5.18		Crippen Method
logp	5.056		Crippen Method
mvol	327.500	ml/mol	McGowan Method
pc	1014.24	kPa	Joback Method
rinpol	3000.00		NIST Webbook
rinpol	3000.00		NIST Webbook
tb	851.65	K	Joback Method
tc	1043.69	K	Joback Method
tf	495.40	K	Joback Method
vc	1.266	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1062.72	J/molxK	851.65	Joback Method
cpg	1081.03	J/molxK	883.66	Joback Method
cpg	1098.15	J/molxK	915.66	Joback Method
cpg	1114.10	J/molxK	947.67	Joback Method
cpg	1128.92	J/molxK	979.68	Joback Method
cpg	1142.62	J/molxK	1011.68	Joback Method
cpg	1155.23	J/molxK	1043.69	Joback Method
dvisc	0.0004724	Paxs	495.40	Joback Method

dvisc	0.0002272	Paxs	554.77	Joback Method
dvisc	0.0001259	Paxs	614.15	Joback Method
dvisc	0.0000774	Paxs	673.52	Joback Method
dvisc	0.0000515	Paxs	732.90	Joback Method
dvisc	0.0000364	Paxs	792.27	Joback Method
dvisc	0.0000271	Paxs	851.65	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=U381924&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
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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