

Diglycolic acid, butyl tridecyl ester

Inchi:	InChI=1S/C21H40O5/c1-3-5-7-8-9-10-11-12-13-14-15-17-26-21(23)19-24-18-20(22)25-1
InchiKey:	VTIMNPSEKHDVHP-UHFFFAOYSA-N
Formula:	C21H40O5
SMILES:	CCCCCCCCCCCCOC(=O)COCC(=O)OCCCC
Mol. weight [g/mol]:	372.54

Physical Properties

Property code	Value	Unit	Source
gf	-446.90	kJ/mol	Joback Method
hf	-1098.59	kJ/mol	Joback Method
hfus	56.91	kJ/mol	Joback Method
hvap	83.06	kJ/mol	Joback Method
log10ws	-5.43		Crippen Method
logp	5.201		Crippen Method
mvol	327.500	ml/mol	McGowan Method
pc	1002.08	kPa	Joback Method
rinpol	3267.00		NIST Webbook
rinpol	3267.00		NIST Webbook
tb	854.88	K	Joback Method
tc	1046.67	K	Joback Method
tf	492.98	K	Joback Method
vc	1.278	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1062.15	J/molxK	854.88	Joback Method
cpg	1080.63	J/molxK	886.84	Joback Method
cpg	1097.88	J/molxK	918.81	Joback Method
cpg	1113.92	J/molxK	950.77	Joback Method
cpg	1128.76	J/molxK	982.74	Joback Method
cpg	1142.41	J/molxK	1014.70	Joback Method
cpg	1154.88	J/molxK	1046.67	Joback Method
dvisc	0.0005115	Paxs	492.98	Joback Method

dvisc	0.0002551	Paxs	553.30	Joback Method
dvisc	0.0001459	Paxs	613.61	Joback Method
dvisc	0.0000922	Paxs	673.93	Joback Method
dvisc	0.0000628	Paxs	734.25	Joback Method
dvisc	0.0000454	Paxs	794.56	Joback Method
dvisc	0.0000343	Paxs	854.88	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381858&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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