

Diglycolic acid, butyl tetradecyl ester

Inchi:	InChI=1S/C22H42O5/c1-3-5-7-8-9-10-11-12-13-14-15-16-18-27-22(24)20-25-19-21(23)2
InchiKey:	FFUDFWNZRZRZFQ-UHFFFAOYSA-N
Formula:	C22H42O5
SMILES:	CCCCCCCCCCCCCOC(=O)COCC(=O)OCCCC
Mol. weight [g/mol]:	386.57

Physical Properties

Property code	Value	Unit	Source
gf	-438.48	kJ/mol	Joback Method
hf	-1119.23	kJ/mol	Joback Method
hfus	59.50	kJ/mol	Joback Method
hvap	85.29	kJ/mol	Joback Method
log10ws	-5.84		Crippen Method
logp	5.591		Crippen Method
mvol	341.590	ml/mol	McGowan Method
pc	943.84	kPa	Joback Method
rinpol	3371.00		NIST Webbook
rinpol	3371.00		NIST Webbook
tb	877.76	K	Joback Method
tc	1074.82	K	Joback Method
tf	504.25	K	Joback Method
vc	1.333	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1124.11	J/molxK	877.76	Joback Method
cpg	1143.04	J/molxK	910.60	Joback Method
cpg	1160.64	J/molxK	943.45	Joback Method
cpg	1176.92	J/molxK	976.29	Joback Method
cpg	1191.91	J/molxK	1009.14	Joback Method
cpg	1205.60	J/molxK	1041.98	Joback Method
cpg	1218.02	J/molxK	1074.82	Joback Method
dvisc	0.0004546	Paxs	504.25	Joback Method

dvisc	0.0002244	Paxs	566.50	Joback Method
dvisc	0.0001273	Paxs	628.75	Joback Method
dvisc	0.0000800	Paxs	691.00	Joback Method
dvisc	0.0000543	Paxs	753.26	Joback Method
dvisc	0.0000391	Paxs	815.51	Joback Method
dvisc	0.0000295	Paxs	877.76	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381847&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

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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