

Diglycolic acid, octyl undecyl ester

Inchi:	InChI=1S/C23H44O5/c1-3-5-7-9-11-12-13-15-17-19-28-23(25)21-26-20-22(24)27-18-16-
InchiKey:	UIVMRQKEWOSAIE-UHFFFAOYSA-N
Formula:	C23H44O5
SMILES:	CCCCCCCCCOC(=O)COCC(=O)OCCCCCCCC
Mol. weight [g/mol]:	400.59

Physical Properties

Property code	Value	Unit	Source
gf	-430.06	kJ/mol	Joback Method
hf	-1139.87	kJ/mol	Joback Method
hfus	62.09	kJ/mol	Joback Method
hvap	87.51	kJ/mol	Joback Method
log10ws	-6.26		Crippen Method
logp	5.981		Crippen Method
mvol	355.680	ml/mol	McGowan Method
pc	890.54	kPa	Joback Method
rinpol	3351.00		NIST Webbook
rinpol	3351.00		NIST Webbook
tb	900.64	K	Joback Method
tc	1103.95	K	Joback Method
tf	515.52	K	Joback Method
vc	1.389	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1186.66	J/molxK	900.64	Joback Method
cpg	1269.34	J/molxK	1070.07	Joback Method
cpg	1255.63	J/molxK	1036.18	Joback Method
cpg	1240.53	J/molxK	1002.30	Joback Method
cpg	1224.02	J/molxK	968.41	Joback Method
cpg	1206.06	J/molxK	934.53	Joback Method
cpg	1281.67	J/molxK	1103.95	Joback Method
dvisc	0.0000253	Paxs	900.64	Joback Method

dvisc	0.0000337	Paxs	836.45	Joback Method
dvisc	0.0000469	Paxs	772.27	Joback Method
dvisc	0.0000693	Paxs	708.08	Joback Method
dvisc	0.0001109	Paxs	643.89	Joback Method
dvisc	0.0001968	Paxs	579.71	Joback Method
dvisc	0.0004027	Paxs	515.52	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382119&Units=SI

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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