

Diglycolic acid, 2-methylbutyl undecyl ester

Inchi:	InChI=1S/C20H38O5/c1-4-6-7-8-9-10-11-12-13-14-24-19(21)16-23-17-20(22)25-15-18(3
InchiKey:	MSSSKVZZDLFOCK-UHFFFAOYSA-N
Formula:	C20H38O5
SMILES:	CCCCCCCCCOC(=O)COCC(=O)OCC(C)CC
Mol. weight [g/mol]:	358.51

Physical Properties

Property code	Value	Unit	Source
gf	-457.76	kJ/mol	Joback Method
hf	-1083.23	kJ/mol	Joback Method
hfus	50.80	kJ/mol	Joback Method
hvap	80.45	kJ/mol	Joback Method
log10ws	-4.77		Crippen Method
logp	4.666		Crippen Method
mvol	313.410	ml/mol	McGowan Method
pc	1071.46	kPa	Joback Method
rinpol	3018.00		NIST Webbook
rinpol	3018.00		NIST Webbook
tb	831.56	K	Joback Method
tc	1019.41	K	Joback Method
tf	466.71	K	Joback Method
vc	1.216	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1001.32	J/molxK	831.56	Joback Method
cpg	1019.40	J/molxK	862.87	Joback Method
cpg	1036.34	J/molxK	894.18	Joback Method
cpg	1052.14	J/molxK	925.48	Joback Method
cpg	1066.81	J/molxK	956.79	Joback Method
cpg	1080.36	J/molxK	988.10	Joback Method
cpg	1092.80	J/molxK	1019.41	Joback Method
dvisc	0.0006668	Paxs	466.71	Joback Method

dvisc	0.0003109	Paxs	527.52	Joback Method
dvisc	0.0001697	Paxs	588.33	Joback Method
dvisc	0.0001037	Paxs	649.13	Joback Method
dvisc	0.0000690	Paxs	709.94	Joback Method
dvisc	0.0000489	Paxs	770.75	Joback Method
dvisc	0.0000365	Paxs	831.56	Joback Method

Sources

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=U381821&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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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