

Diglycolic acid, heptyl propyl ester

Inchi:	InChI=1S/C14H26O5/c1-3-5-6-7-8-10-19-14(16)12-17-11-13(15)18-9-4-2/h3-12H2,1-2H3
InchiKey:	GCJOZGDXTFC DLC-UHFFFAOYSA-N
Formula:	C14H26O5
SMILES:	CCCCCCCOC(=O)COCC(=O)OCCC
Mol. weight [g/mol]:	274.35

Physical Properties

Property code	Value	Unit	Source
gf	-505.84	kJ/mol	Joback Method
hf	-954.11	kJ/mol	Joback Method
hfus	38.78	kJ/mol	Joback Method
hvap	67.48	kJ/mol	Joback Method
log10ws	-2.50		Crippen Method
logp	2.470		Crippen Method
mvol	228.870	ml/mol	McGowan Method
pc	1616.77	kPa	Joback Method
rinpol	2270.00		NIST Webbook
rinpol	2270.00		NIST Webbook
tb	694.72	K	Joback Method
tc	871.11	K	Joback Method
tf	414.09	K	Joback Method
vc	0.885	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	651.00	J/molxK	694.72	Joback Method
cpg	720.92	J/molxK	841.71	Joback Method
cpg	708.43	J/molxK	812.31	Joback Method
cpg	695.18	J/molxK	782.91	Joback Method
cpg	681.20	J/molxK	753.52	Joback Method
cpg	666.47	J/molxK	724.12	Joback Method
cpg	732.66	J/molxK	871.11	Joback Method
dvisc	0.0000920	Paxs	694.72	Joback Method

dvisc	0.0001192	Paxs	647.95	Joback Method
dvisc	0.0001607	Paxs	601.18	Joback Method
dvisc	0.0002278	Paxs	554.40	Joback Method
dvisc	0.0003444	Paxs	507.63	Joback Method
dvisc	0.0005663	Paxs	460.86	Joback Method
dvisc	0.0010418	Paxs	414.09	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381952&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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