

Diglycolic acid, heptyl 3-methylpent-2-yl ester

Inchi:	InChI=1S/C17H32O5/c1-5-7-8-9-10-11-21-16(18)12-20-13-17(19)22-15(4)14(3)6-2/h14-1
InchiKey:	ZMIHCUFBOPDSGG-UHFFFAOYSA-N
Formula:	C17H32O5
SMILES:	CCCCCCCOC(=O)COCC(=O)OC(C)C(C)CC
Mol. weight [g/mol]:	316.43

Physical Properties

Property code	Value	Unit	Source
gf	-485.46	kJ/mol	Joback Method
hf	-1026.59	kJ/mol	Joback Method
hfus	39.50	kJ/mol	Joback Method
hvap	73.38	kJ/mol	Joback Method
log10ws	-3.62		Crippen Method
logp	3.494		Crippen Method
mvol	271.140	ml/mol	McGowan Method
pc	1313.70	kPa	Joback Method
rinpol	2533.00		NIST Webbook
rinpol	2533.00		NIST Webbook
tb	762.48	K	Joback Method
tc	944.32	K	Joback Method
tf	417.90	K	Joback Method
vc	1.042	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	822.56	J/molxK	762.48	Joback Method
cpg	839.65	J/molxK	792.79	Joback Method
cpg	855.78	J/molxK	823.09	Joback Method
cpg	870.96	J/molxK	853.40	Joback Method
cpg	885.19	J/molxK	883.71	Joback Method
cpg	898.47	J/molxK	914.02	Joback Method
cpg	910.80	J/molxK	944.32	Joback Method
dvisc	0.0011284	Paxs	417.90	Joback Method

dvisc	0.0004957	Paxs	475.33	Joback Method
dvisc	0.0002600	Paxs	532.76	Joback Method
dvisc	0.0001546	Paxs	590.19	Joback Method
dvisc	0.0001008	Paxs	647.62	Joback Method
dvisc	0.0000705	Paxs	705.05	Joback Method
dvisc	0.0000520	Paxs	762.48	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=U381875&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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