

Diglycolic acid, 2-methylphenyl pentyl ester

Inchi:	InChI=1S/C16H22O5/c1-3-4-7-10-20-15(17)11-19-12-16(18)21-14-9-6-5-8-13(14)2/h5-6,
InchiKey:	UVKOGUXUOLGGHO-UHFFFAOYSA-N
Formula:	C16H22O5
SMILES:	CCCCCOC(=O)COCC(=O)Oc1ccccc1C
Mol. weight [g/mol]:	294.34

Physical Properties

Property code	Value	Unit	Source
gf	-386.22	kJ/mol	Joback Method
hf	-770.33	kJ/mol	Joback Method
hfus	37.61	kJ/mol	Joback Method
hvap	74.87	kJ/mol	Joback Method
log10ws	-3.14		Crippen Method
logp	2.650		Crippen Method
mcvol	233.290	ml/mol	McGowan Method
pc	1790.91	kPa	Joback Method
rinsol	2760.00		NIST Webbook
tb	772.14	K	Joback Method
tc	973.24	K	Joback Method
tf	475.57	K	Joback Method
vc	0.889	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	676.30	J/molxK	772.14	Joback Method
cpg	691.04	J/molxK	805.66	Joback Method
cpg	704.79	J/molxK	839.17	Joback Method
cpg	717.53	J/molxK	872.69	Joback Method
cpg	729.27	J/molxK	906.21	Joback Method
cpg	739.99	J/molxK	939.73	Joback Method
cpg	749.72	J/molxK	973.24	Joback Method
dvisc	0.0006097	Paxs	475.57	Joback Method
dvisc	0.0003602	Paxs	525.00	Joback Method

dvisc	0.0002330	Paxs	574.43	Joback Method
dvisc	0.0001615	Paxs	623.86	Joback Method
dvisc	0.0001181	Paxs	673.28	Joback Method
dvisc	0.0000902	Paxs	722.71	Joback Method
dvisc	0.0000713	Paxs	772.14	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382007&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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
rinpolar:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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