

Diglycolic acid, 2-acetylphenyl isobutyl ester

Inchi:	InChI=1S/C16H20O6/c1-11(2)8-21-15(18)9-20-10-16(19)22-14-7-5-4-6-13(14)12(3)17/h4
InchiKey:	QAUGPIHZWRDTDY-UHFFFAOYSA-N
Formula:	C16H20O6
SMILES:	CC(=O)c1ccccc1OC(=O)COCC(=O)OCC(C)C
Mol. weight [g/mol]:	308.33

Physical Properties

Property code	Value	Unit	Source
gf	-517.58	kJ/mol	Joback Method
hf	-888.19	kJ/mol	Joback Method
hfus	35.69	kJ/mol	Joback Method
hvap	81.23	kJ/mol	Joback Method
log10ws	-2.67		Crippen Method
logp	2.010		Crippen Method
mcvol	234.860	ml/mol	McGowan Method
pc	1903.58	kPa	Joback Method
rinpol	2538.00		NIST Webbook
rinpol	2538.00		NIST Webbook
tb	825.57	K	Joback Method
tc	1036.05	K	Joback Method
tf	510.50	K	Joback Method
vc	0.889	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	691.98	J/molxK	825.57	Joback Method
cpg	705.14	J/molxK	860.65	Joback Method
cpg	717.18	J/molxK	895.73	Joback Method
cpg	728.10	J/molxK	930.81	Joback Method
cpg	737.88	J/molxK	965.89	Joback Method
cpg	746.54	J/molxK	1000.97	Joback Method
cpg	754.05	J/molxK	1036.05	Joback Method
dvisc	0.0005715	Paxs	510.50	Joback Method

dvisc	0.0003339	Paxs	563.01	Joback Method
dvisc	0.0002138	Paxs	615.52	Joback Method
dvisc	0.0001468	Paxs	668.03	Joback Method
dvisc	0.0001065	Paxs	720.55	Joback Method
dvisc	0.0000807	Paxs	773.06	Joback Method
dvisc	0.0000634	Paxs	825.57	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=U382718&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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