Diglycolic acid, 2-acetylphenyl isohexyl ester

Inchi: InChI=1S/C18H24O6/c1-13(2)7-6-10-23-17(20)11-22-12-18(21)24-16-9-5-4-8-15(16)14(3
InchiKey: BDWFCNCVTQZKCP-UHFFFAOYSA-N
Formula: C18H24O6
SMILES: CC(=O)c1ccccc1OC(=O)COCC(=O)OCCCC(C)C
Mol. weight [g/mol]: 336.38

Physical Properties

Property code	Value	Unit	Source
gf	-500.74	kJ/mol	Joback Method
hf	-929.47	kJ/mol	Joback Method
hfus	40.87	kJ/mol	Joback Method
hvap	85.68	kJ/mol	Joback Method
log10ws	-3.50		Crippen Method
logp	2.791		Crippen Method
mcvol	263.040	ml/mol	McGowan Method
pc	1620.68	kPa	Joback Method
rinpol	2844.00		NIST Webbook
rinpol	2844.00		NIST Webbook
tb	871.33	K	Joback Method
tc	1080.93	K	Joback Method
tf	533.04	K	Joback Method
vc	1.002	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	805.80	J/mol×K	871.33	Joback Method
cpg	819.31	J/mol×K	906.26	Joback Method
cpg	831.59	J/mol×K	941.20	Joback Method
cpg	842.64	J/mol×K	976.13	Joback Method
cpg	852.48	J/mol×K	1011.06	Joback Method
cpg	861.10	J/mol×K	1046.00	Joback Method
cpg	868.50	J/mol×K	1080.93	Joback Method
dvisc	0.0004673	Pa×s	533.04	Joback Method

dvisc	0.0002665	Pa×s	589.42	Joback Method
dvisc	0.0001676	Pa×s	645.80	Joback Method
dvisc	0.0001136	Pa×s	702.18	Joback Method
dvisc	0.0000815	Pa×s	758.57	Joback Method
dvisc	0.0000613	Pa×s	814.95	Joback Method
dvisc	0.0000478	Pa×s	871.33	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382721&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
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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