

Succinic acid, hexyl 3-iodobenzyl ester

Inchi: InChI=1S/C17H23IO4/c1-2-3-4-5-11-21-16(19)9-10-17(20)22-13-14-7-6-8-15(18)12-14/h
InchiKey: BWQHKFGXXBOXTD-UHFFFAOYSA-N
Formula: C17H23IO4
SMILES: CCCCCCOC(=O)CCC(=O)OCc1cccc(I)c1
Mol. weight [g/mol]: 418.27

Physical Properties

Property code	Value	Unit	Source
gf	-214.68	kJ/mol	Joback Method
hf	-581.88	kJ/mol	Joback Method
hfus	43.42	kJ/mol	Joback Method
hvap	84.06	kJ/mol	Joback Method
log10ws	-5.41		Crippen Method
logp	4.238		Crippen Method
mvol	267.330	ml/mol	McGowan Method
pc	1647.09	kPa	Joback Method
rinpol	2546.00		NIST Webbook
rinpol	2546.00		NIST Webbook
tb	865.74	K	Joback Method
tc	1085.74	K	Joback Method
tf	522.67	K	Joback Method
vc	1.016	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	755.15	J/molxK	865.74	Joback Method
cpg	811.59	J/molxK	1049.07	Joback Method
cpg	802.37	J/molxK	1012.41	Joback Method
cpg	792.14	J/molxK	975.74	Joback Method
cpg	780.88	J/molxK	939.07	Joback Method
cpg	768.56	J/molxK	902.41	Joback Method
cpg	819.86	J/molxK	1085.74	Joback Method
dvisc	0.0000608	Paxs	865.74	Joback Method

dvisc	0.0000775	Paxs	808.56	Joback Method
dvisc	0.0001027	Paxs	751.38	Joback Method
dvisc	0.0001424	Paxs	694.20	Joback Method
dvisc	0.0002095	Paxs	637.03	Joback Method
dvisc	0.0003326	Paxs	579.85	Joback Method
dvisc	0.0005842	Paxs	522.67	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=U381386&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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