

Succinic acid, 2-iodobenzyl isobutyl ester

Inchi: InChI=1S/C15H19IO4/c1-11(2)9-19-14(17)7-8-15(18)20-10-12-5-3-4-6-13(12)16/h3-6,11
InchiKey: LQRUKECWYVWSBZ-UHFFFAOYSA-N
Formula: C15H19IO4
SMILES: CC(C)COC(=O)CCC(=O)OCc1ccccc1I
Mol. weight [g/mol]: 390.21

Physical Properties

Property code	Value	Unit	Source
gf	-233.96	kJ/mol	Joback Method
hf	-545.88	kJ/mol	Joback Method
hfus	34.71	kJ/mol	Joback Method
hvap	79.22	kJ/mol	Joback Method
log10ws	-4.33		Crippen Method
logp	3.314		Crippen Method
mvol	239.150	ml/mol	McGowan Method
pc	1950.95	kPa	Joback Method
rinpol	2296.00		NIST Webbook
rinpol	2296.00		NIST Webbook
tb	819.54	K	Joback Method
tc	1046.98	K	Joback Method
tf	485.13	K	Joback Method
vc	0.897	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	643.48	J/molxK	819.54	Joback Method
cpg	656.58	J/molxK	857.45	Joback Method
cpg	668.60	J/molxK	895.35	Joback Method
cpg	679.56	J/molxK	933.26	Joback Method
cpg	689.49	J/molxK	971.17	Joback Method
cpg	698.42	J/molxK	1009.07	Joback Method
cpg	706.37	J/molxK	1046.98	Joback Method
dvisc	0.0008096	Paxs	485.13	Joback Method

dvisc	0.0004434	Paxs	540.87	Joback Method
dvisc	0.0002717	Paxs	596.60	Joback Method
dvisc	0.0001811	Paxs	652.34	Joback Method
dvisc	0.0001286	Paxs	708.07	Joback Method
dvisc	0.0000960	Paxs	763.80	Joback Method
dvisc	0.0000746	Paxs	819.54	Joback Method

Sources

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=U381101&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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