

Succinic acid, 4-iodobenzyl 2-methylhex-3-yl ester

Inchi:	InChI=1S/C18H25IO4/c1-4-5-16(13(2)3)23-18(21)11-10-17(20)22-12-14-6-8-15(19)9-7-1
InchiKey:	HUMOIHSHRDDJRX-UHFFFAOYSA-N
Formula:	C18H25IO4
SMILES:	CCCC(OC(=O)CCC(=O)OCc1ccc(I)cc1)C(C)C
Mol. weight [g/mol]:	432.29

Physical Properties

Property code	Value	Unit	Source
gf	-211.14	kJ/mol	Joback Method
hf	-613.08	kJ/mol	Joback Method
hfus	38.96	kJ/mol	Joback Method
hvap	85.51	kJ/mol	Joback Method
log10ws	-5.70		Crippen Method
logp	4.483		Crippen Method
mvol	281.420	ml/mol	McGowan Method
pc	1545.13	kPa	Joback Method
rinpol	2521.00		NIST Webbook
rinpol	2521.00		NIST Webbook
tb	887.74	K	Joback Method
tc	1111.68	K	Joback Method
tf	503.94	K	Joback Method
vc	1.060	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	813.61	J/molxK	887.74	Joback Method
cpg	827.46	J/molxK	925.06	Joback Method
cpg	840.11	J/molxK	962.39	Joback Method
cpg	851.60	J/molxK	999.71	Joback Method
cpg	861.97	J/molxK	1037.04	Joback Method
cpg	871.24	J/molxK	1074.36	Joback Method
cpg	879.47	J/molxK	1111.68	Joback Method
dvisc	0.0006556	Paxs	503.94	Joback Method

dvisc	0.0003239	Paxs	567.91	Joback Method
dvisc	0.0001845	Paxs	631.87	Joback Method
dvisc	0.0001166	Paxs	695.84	Joback Method
dvisc	0.0000796	Paxs	759.81	Joback Method
dvisc	0.0000577	Paxs	823.77	Joback Method
dvisc	0.0000438	Paxs	887.74	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=U380893&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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