

Sebacic acid, 3-iodobenzyl propyl ester

Inchi: InChI=1S/C20H29IO4/c1-2-14-24-19(22)12-7-5-3-4-6-8-13-20(23)25-16-17-10-9-11-18(2)
InchiKey: XHBLQCFLMYSVRA-UHFFFAOYSA-N
Formula: C20H29IO4
SMILES: CCCOC(=O)CCCCCCCCC(=O)OCc1cccc(I)c1
Mol. weight [g/mol]: 460.35

Physical Properties

Property code	Value	Unit	Source
gf	-189.42	kJ/mol	Joback Method
hf	-643.80	kJ/mol	Joback Method
hfus	51.19	kJ/mol	Joback Method
hvap	90.74	kJ/mol	Joback Method
log10ws	-6.67		Crippen Method
logp	5.408		Crippen Method
mvol	309.600	ml/mol	McGowan Method
pc	1320.39	kPa	Joback Method
rinpol	2890.00		NIST Webbook
rinpol	2890.00		NIST Webbook
tb	934.38	K	Joback Method
tc	1153.60	K	Joback Method
tf	556.48	K	Joback Method
vc	1.183	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	929.57	J/molxK	934.38	Joback Method
cpg	987.92	J/molxK	1117.07	Joback Method
cpg	978.46	J/molxK	1080.53	Joback Method
cpg	967.93	J/molxK	1043.99	Joback Method
cpg	956.30	J/molxK	1007.45	Joback Method
cpg	943.53	J/molxK	970.92	Joback Method
cpg	996.37	J/molxK	1153.60	Joback Method
dvisc	0.0000387	Paxs	934.38	Joback Method

dvisc	0.0000498	Paxs	871.40	Joback Method
dvisc	0.0000667	Paxs	808.41	Joback Method
dvisc	0.0000938	Paxs	745.43	Joback Method
dvisc	0.0001406	Paxs	682.45	Joback Method
dvisc	0.0002288	Paxs	619.46	Joback Method
dvisc	0.0004156	Paxs	556.48	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=U380752&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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