

Sebacic acid, ethyl 3-iodobenzyl ester

Inchi:	InChI=1S/C19H27IO4/c1-2-23-18(21)12-7-5-3-4-6-8-13-19(22)24-15-16-10-9-11-17(20)1
InchiKey:	JXXZFUMENFUHPR-UHFFFAOYSA-N
Formula:	C19H27IO4
SMILES:	CCOC(=O)CCCCCCCC(=O)OCc1cccc(I)c1
Mol. weight [g/mol]:	446.32

Physical Properties

Property code	Value	Unit	Source
gf	-197.84	kJ/mol	Joback Method
hf	-623.16	kJ/mol	Joback Method
hfus	48.60	kJ/mol	Joback Method
hvap	88.51	kJ/mol	Joback Method
log10ws	-6.25		Crippen Method
logp	5.018		Crippen Method
mcvol	295.510	ml/mol	McGowan Method
pc	1417.57	kPa	Joback Method
rinqol	2794.00		NIST Webbook
tb	911.50	K	Joback Method
tc	1130.22	K	Joback Method
tf	545.21	K	Joback Method
vc	1.127	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	870.71	J/molxK	911.50	Joback Method
cpg	928.52	J/molxK	1093.76	Joback Method
cpg	919.11	J/molxK	1057.31	Joback Method
cpg	908.66	J/molxK	1020.86	Joback Method
cpg	897.14	J/molxK	984.41	Joback Method
cpg	884.50	J/molxK	947.95	Joback Method
cpg	936.92	J/molxK	1130.22	Joback Method
dvisc	0.0000450	Paxs	911.50	Joback Method
dvisc	0.0000578	Paxs	850.45	Joback Method

dvisc	0.0000772	Paxs	789.40	Joback Method
dvisc	0.0001081	Paxs	728.36	Joback Method
dvisc	0.0001610	Paxs	667.31	Joback Method
dvisc	0.0002599	Paxs	606.26	Joback Method
dvisc	0.0004671	Paxs	545.21	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380751&Units=SI
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

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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