

Sebacic acid, 3-hexyl isobutyl ester

Inchi:	InChI=1S/C20H38O4/c1-5-13-18(6-2)24-20(22)15-12-10-8-7-9-11-14-19(21)23-16-17(3)-
InchiKey:	JZWBZGUYIHGQFH-UHFFFAOYSA-N
Formula:	C20H38O4
SMILES:	CCCC(CC)OC(=O)CCCCCCCCC(=O)OCC(C)C
Mol. weight [g/mol]:	342.51

Physical Properties

Property code	Value	Unit	Source
gf	-355.20	kJ/mol	Joback Method
hf	-956.29	kJ/mol	Joback Method
hfus	46.08	kJ/mol	Joback Method
hvap	77.65	kJ/mol	Joback Method
log10ws	-5.79		Crippen Method
logp	5.428		Crippen Method
mvol	307.540	ml/mol	McGowan Method
pc	1089.22	kPa	Joback Method
rinpol	2252.00		NIST Webbook
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tb	808.70	K	Joback Method
tc	994.02	K	Joback Method
tf	429.48	K	Joback Method
vc	1.192	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	970.14	J/molxK	808.70	Joback Method
cpg	988.55	J/molxK	839.59	Joback Method
cpg	1005.89	J/molxK	870.47	Joback Method
cpg	1022.17	J/molxK	901.36	Joback Method
cpg	1037.40	J/molxK	932.24	Joback Method
cpg	1051.61	J/molxK	963.13	Joback Method
cpg	1064.82	J/molxK	994.02	Joback Method
dvisc	0.0011959	Paxs	429.48	Joback Method

dvisc	0.0004873	Paxs	492.68	Joback Method
dvisc	0.0002435	Paxs	555.89	Joback Method
dvisc	0.0001402	Paxs	619.09	Joback Method
dvisc	0.0000894	Paxs	682.29	Joback Method
dvisc	0.0000615	Paxs	745.50	Joback Method
dvisc	0.0000449	Paxs	808.70	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355538&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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