

Sebacic acid, isohexyl 3-methylbutyl ester

Inchi:	InChI=1S/C21H40O4/c1-18(2)12-11-16-24-20(22)13-9-7-5-6-8-10-14-21(23)25-17-15-19
InchiKey:	KIDGODGHYCHNQH-UHFFFAOYSA-N
Formula:	C21H40O4
SMILES:	CC(C)CCCOC(=O)CCCCCCCCC(=O)OCCC(C)C
Mol. weight [g/mol]:	356.54

Physical Properties

Property code	Value	Unit	Source
gf	-346.78	kJ/mol	Joback Method
hf	-976.93	kJ/mol	Joback Method
hfus	48.67	kJ/mol	Joback Method
hvap	79.88	kJ/mol	Joback Method
log10ws	-5.85		Crippen Method
logp	5.676		Crippen Method
mvol	321.630	ml/mol	McGowan Method
pc	1023.34	kPa	Joback Method
rmpol	2414.00		NIST Webbook
tb	831.58	K	Joback Method
tc	1019.89	K	Joback Method
tf	440.75	K	Joback Method
vc	1.248	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1031.20	J/molxK	831.58	Joback Method
cpg	1113.87	J/molxK	988.51	Joback Method
cpg	1099.54	J/molxK	957.12	Joback Method
cpg	1084.13	J/molxK	925.74	Joback Method
cpg	1067.62	J/molxK	894.35	Joback Method
cpg	1049.98	J/molxK	862.97	Joback Method
cpg	1127.14	J/molxK	1019.89	Joback Method
dvisc	0.0000387	Paxs	831.58	Joback Method
dvisc	0.0000532	Paxs	766.44	Joback Method

dvisc	0.0000774	Paxs	701.30	Joback Method
dvisc	0.0001217	Paxs	636.16	Joback Method
dvisc	0.0002123	Paxs	571.03	Joback Method
dvisc	0.0004270	Paxs	505.89	Joback Method
dvisc	0.0010562	Paxs	440.75	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=U355369&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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