

Sebacic acid, isohexyl 2-methylpent-3-yl ester

Inchi: InChI=1S/C22H42O4/c1-6-20(19(4)5)26-22(24)16-12-10-8-7-9-11-15-21(23)25-17-13-14
InchiKey: XLBQPZFXVRZNLK-UHFFFAOYSA-N
Formula: C22H42O4
SMILES: CCC(OC(=O)CCCCCCCC(=O)OCCCC(C)C)C(C)C
Mol. weight [g/mol]: 370.57

Physical Properties

Property code	Value	Unit	Source
gf	-340.80	kJ/mol	Joback Method
hf	-1002.85	kJ/mol	Joback Method
hfus	47.74	kJ/mol	Joback Method
hvap	81.71	kJ/mol	Joback Method
log10ws	-6.39		Crippen Method
logp	6.064		Crippen Method
mvol	335.720	ml/mol	McGowan Method
pc	968.07	kPa	Joback Method
rinpol	2435.00		NIST Webbook
rinpol	2435.00		NIST Webbook
tb	854.02	K	Joback Method
tc	1046.45	K	Joback Method
tf	437.02	K	Joback Method
vc	1.298	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1093.43	J/molxK	854.02	Joback Method
cpg	1112.63	J/molxK	886.09	Joback Method
cpg	1130.59	J/molxK	918.16	Joback Method
cpg	1147.34	J/molxK	950.24	Joback Method
cpg	1162.90	J/molxK	982.31	Joback Method
cpg	1177.30	J/molxK	1014.38	Joback Method
cpg	1190.56	J/molxK	1046.45	Joback Method
dvisc	0.0011301	Paxs	437.02	Joback Method

dvisc	0.0004097	Paxs	506.52	Joback Method
dvisc	0.0001897	Paxs	576.02	Joback Method
dvisc	0.0001037	Paxs	645.52	Joback Method
dvisc	0.0000637	Paxs	715.02	Joback Method
dvisc	0.0000427	Paxs	784.52	Joback Method
dvisc	0.0000305	Paxs	854.02	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=U355453&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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