

Sebacic acid, isohexyl undecyl ester

Inchi: InChI=1S/C27H52O4/c1-4-5-6-7-8-9-12-15-18-23-30-26(28)21-16-13-10-11-14-17-22-27
InchiKey: FQNFTKFTIYCEGY-UHFFFAOYSA-N
Formula: C27H52O4
SMILES: CCCCCCCCCCOC(=O)CCCCCCCCC(=O)OCCCC(C)C
Mol. weight [g/mol]: 440.70

Physical Properties

Property code	Value	Unit	Source
gf	-293.82	kJ/mol	Joback Method
hf	-1095.49	kJ/mol	Joback Method
hfus	67.74	kJ/mol	Joback Method
hvap	93.62	kJ/mol	Joback Method
log10ws	-8.61		Crippen Method
logp	8.161		Crippen Method
mvol	406.170	ml/mol	McGowan Method
pc	726.53	kPa	Joback Method
rinpol	3087.00		NIST Webbook
rinpol	3087.00		NIST Webbook
tb	969.30	K	Joback Method
tc	1196.72	K	Joback Method
tf	523.37	K	Joback Method
vc	1.589	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1410.04	J/molxK	969.30	Joback Method
cpg	1501.39	J/molxK	1158.81	Joback Method
cpg	1486.55	J/molxK	1120.91	Joback Method
cpg	1470.06	J/molxK	1083.01	Joback Method
cpg	1451.85	J/molxK	1045.11	Joback Method
cpg	1431.86	J/molxK	1007.20	Joback Method
cpg	1514.63	J/molxK	1196.72	Joback Method
dvisc	0.0000168	Paxs	969.30	Joback Method

dvisc	0.0000230	Paxs	894.98	Joback Method
dvisc	0.0000331	Paxs	820.66	Joback Method
dvisc	0.0000515	Paxs	746.34	Joback Method
dvisc	0.0000881	Paxs	672.01	Joback Method
dvisc	0.0001723	Paxs	597.69	Joback Method
dvisc	0.0004080	Paxs	523.37	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=U354283&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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