

Sebacic acid, 3,3-dimethylbut-2-yl octyl ester

Inchi:	InChI=1S/C24H46O4/c1-6-7-8-9-14-17-20-27-22(25)18-15-12-10-11-13-16-19-23(26)28-
InchiKey:	XOAZEUKLDBXMSN-UHFFFAOYSA-N
Formula:	C24H46O4
SMILES:	CCCCCCCCOC(=O)CCCCCCCC(=O)OC(C)C(C)C(C)C
Mol. weight [g/mol]:	398.62

Physical Properties

Property code	Value	Unit	Source
gf	-316.24	kJ/mol	Joback Method
hf	-1042.32	kJ/mol	Joback Method
hfus	52.55	kJ/mol	Joback Method
hvap	85.65	kJ/mol	Joback Method
log10ws	-7.46		Crippen Method
logp	6.989		Crippen Method
mcvol	363.900	ml/mol	McGowan Method
pc	863.53	kPa	Joback Method
rinqol	2645.00		NIST Webbook
tb	897.43	K	Joback Method
tc	1098.73	K	Joback Method
tf	491.98	K	Joback Method
vc	1.411	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1218.06	J/molxK	897.43	Joback Method
cpg	1304.43	J/molxK	1065.18	Joback Method
cpg	1289.60	J/molxK	1031.63	Joback Method
cpg	1273.61	J/molxK	998.08	Joback Method
cpg	1256.38	J/molxK	964.53	Joback Method
cpg	1237.89	J/molxK	930.98	Joback Method
cpg	1318.12	J/molxK	1098.73	Joback Method
dvisc	0.0000209	Paxs	897.43	Joback Method
dvisc	0.0000289	Paxs	829.86	Joback Method

dvisc	0.0000424	Paxs	762.28	Joback Method
dvisc	0.0000670	Paxs	694.71	Joback Method
dvisc	0.0001168	Paxs	627.13	Joback Method
dvisc	0.0002329	Paxs	559.56	Joback Method
dvisc	0.0005616	Paxs	491.98	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355602&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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