

Sebacic acid, dodecyl 5-methoxy-3-methylpentyl ester

Inchi:	InChI=1S/C29H56O5/c1-4-5-6-7-8-9-10-13-16-19-24-33-28(30)20-17-14-11-12-15-18-21
InchiKey:	JXCFIDBWFVOZOD-UHFFFAOYSA-N
Formula:	C29H56O5
SMILES:	CCCCCCCCCCCCOC(=O)CCCCCCCC(=O)OCCC(C)CCOC
Mol. weight [g/mol]:	484.75

Physical Properties

Property code	Value	Unit	Source
gf	-381.98	kJ/mol	Joback Method
hf	-1268.99	kJ/mol	Joback Method
hfus	74.10	kJ/mol	Joback Method
hvap	100.48	kJ/mol	Joback Method
log10ws	-8.53		Crippen Method
logp	8.177		Crippen Method
mcvol	440.220	ml/mol	McGowan Method
pc	651.10	kPa	Joback Method
rinpol	3356.00		NIST Webbook
tb	1037.48	K	Joback Method
tc	1300.17	K	Joback Method
tf	568.14	K	Joback Method
vc	1.720	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1570.96	J/molxK	1037.48	Joback Method
cpg	1593.43	J/molxK	1081.26	Joback Method
cpg	1613.23	J/molxK	1125.04	Joback Method
cpg	1630.43	J/molxK	1168.83	Joback Method
cpg	1645.12	J/molxK	1212.61	Joback Method
cpg	1657.35	J/molxK	1256.39	Joback Method
cpg	1667.22	J/molxK	1300.17	Joback Method
dvisc	0.0002050	Paxs	568.14	Joback Method
dvisc	0.0000886	Paxs	646.36	Joback Method

dvisc	0.0000459	Paxs	724.59	Joback Method
dvisc	0.0000270	Paxs	802.81	Joback Method
dvisc	0.0000175	Paxs	881.03	Joback Method
dvisc	0.0000121	Paxs	959.26	Joback Method
dvisc	0.0000089	Paxs	1037.48	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=U355510&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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