

Sebacic acid, tetrahydrofurfuryl tetradecyl ester

Inchi:	InChI=1S/C29H54O5/c1-2-3-4-5-6-7-8-9-10-13-16-19-24-33-28(30)22-17-14-11-12-15-18
InchiKey:	JHCFILMPRSKGKK-UHFFFAOYSA-N
Formula:	C29H54O5
SMILES:	CCCCCCCCCCCCCOC(=O)CCCCCCCC(=O)OCC1CCCO1
Mol. weight [g/mol]:	482.74

Physical Properties

Property code	Value	Unit	Source
gf	-324.11	kJ/mol	Joback Method
hf	-1203.01	kJ/mol	Joback Method
hfus	78.35	kJ/mol	Joback Method
hvap	103.23	kJ/mol	Joback Method
log10ws	-8.78		Crippen Method
logp	8.074		Crippen Method
mvol	429.360	ml/mol	McGowan Method
pc	715.30	kPa	Joback Method
rinpol	3548.00		NIST Webbook
tb	1057.73	K	Joback Method
tc	1314.07	K	Joback Method
tf	598.38	K	Joback Method
vc	1.669	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1565.71	J/molxK	1057.73	Joback Method
cpg	1586.84	J/molxK	1100.45	Joback Method
cpg	1605.69	J/molxK	1143.18	Joback Method
cpg	1622.37	J/molxK	1185.90	Joback Method
cpg	1636.99	J/molxK	1228.62	Joback Method
cpg	1649.66	J/molxK	1271.35	Joback Method
cpg	1660.49	J/molxK	1314.07	Joback Method
dvisc	0.0002904	Paxs	598.38	Joback Method
dvisc	0.0001383	Paxs	674.94	Joback Method

dvisc	0.0000766	Paxs	751.50	Joback Method
dvisc	0.0000473	Paxs	828.06	Joback Method
dvisc	0.0000317	Paxs	904.61	Joback Method
dvisc	0.0000226	Paxs	981.17	Joback Method
dvisc	0.0000169	Paxs	1057.73	Joback Method

Sources

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=U355730&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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