

Sebacic acid, 3-oxobut-2-yl pentadecyl ester

Inchi:	InChI=1S/C29H54O5/c1-4-5-6-7-8-9-10-11-12-13-16-19-22-25-33-28(31)23-20-17-14-15
InchiKey:	PNAVDPAJKIKXKH-UHFFFAOYSA-N
Formula:	C29H54O5
SMILES:	CCCCCCCCCCCCCOC(=O)CCCCCCCC(=O)OC(C)C(C)=O
Mol. weight [g/mol]:	482.74

Physical Properties

Property code	Value	Unit	Source
gf	-405.90	kJ/mol	Joback Method
hf	-1249.35	kJ/mol	Joback Method
hfus	74.52	kJ/mol	Joback Method
hvap	104.82	kJ/mol	Joback Method
log10ws	-9.08		Crippen Method
logp	8.262		Crippen Method
mcvol	435.920	ml/mol	McGowan Method
pc	678.52	kPa	Joback Method
rinpol	3364.00		NIST Webbook
tb	1068.93	K	Joback Method
tc	1340.66	K	Joback Method
tf	595.84	K	Joback Method
vc	1.708	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1557.29	J/molxK	1068.93	Joback Method
cpg	1638.30	J/molxK	1295.37	Joback Method
cpg	1626.75	J/molxK	1250.08	Joback Method
cpg	1612.99	J/molxK	1204.79	Joback Method
cpg	1596.90	J/molxK	1159.51	Joback Method
cpg	1578.37	J/molxK	1114.22	Joback Method
cpg	1647.73	J/molxK	1340.66	Joback Method
dvisc	0.0000113	Paxs	1068.93	Joback Method
dvisc	0.0000153	Paxs	990.08	Joback Method

dvisc	0.0000218	Paxs	911.23	Joback Method
dvisc	0.0000332	Paxs	832.38	Joback Method
dvisc	0.0000553	Paxs	753.54	Joback Method
dvisc	0.0001039	Paxs	674.69	Joback Method
dvisc	0.0002304	Paxs	595.84	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355786&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

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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