Sebacic acid, 4-methylpent-2-yl pentadecyl ester

Inchi: InChI=1S/C31H60O4/c1-5-6-7-8-9-10-11-12-13-14-17-20-23-26-34-30(32)24-21-18-15-1
InchiKey: XNUSQTWLBJMXNV-UHFFFAOYSA-N
Formula: C31H60O4
SMILES: CCCCCCCCCCCCCCCOC(=O)CCCCCCCCC(=O)OC(C)CC(C)C
Mol. weight [g/mol]: 496.81

Physical Properties

Property code	Value	Unit	Source
gf	-262.58	kJ/mol	Joback Method
hf	-1183.33	kJ/mol	Joback Method
hfus	74.57	kJ/mol	Joback Method
hvap	102.14	kJ/mol	Joback Method
log10ws	-10.39		Crippen Method
logp	9.719		Crippen Method
mcvol	462.530	ml/mol	McGowan Method
pc	598.97	kPa	Joback Method
rinpol	3340.00		NIST Webbook
tb	1060.38	K	Joback Method
tc	1335.48	K	Joback Method
tf	553.45	K	Joback Method
vc	1.808	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1671.19	J/mol×K	1060.38	Joback Method
cpg	1695.52	J/mol×K	1106.23	Joback Method
cpg	1717.12	J/mol×K	1152.08	Joback Method
cpg	1736.12	J/mol×K	1197.93	Joback Method
cpg	1752.66	J/mol×K	1243.78	Joback Method
cpg	1766.86	J/mol×K	1289.63	Joback Method
cpg	1778.86	J/mol×K	1335.48	Joback Method
dvisc	0.0002633	Pa×s	553.45	Joback Method
dvisc	0.0001001	Pa×s	637.94	Joback Method

dvisc	0.0000477	Pa×s	722.43	Joback Method
dvisc	0.0000266	Pa×s	806.91	Joback Method
dvisc	0.0000165	Pa×s	891.40	Joback Method
dvisc	0.0000112	Pa×s	975.89	Joback Method
dvisc	0.0000080	Pa×s	1060.38	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355362&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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