

Sebacic acid, heptadecyl oct-3-yl ester

Inchi:	InChI=1S/C35H68O4/c1-4-7-9-10-11-12-13-14-15-16-17-18-21-24-28-32-38-34(36)30-26
InchiKey:	SZNNMNOHVUFBQT-UHFFFAOYSA-N
Formula:	C35H68O4
SMILES:	CCCCCCCCCCCCCCCCOC(=O)CCCCCCCC(=O)OC(CC)CCCC
Mol. weight [g/mol]:	552.91

Physical Properties

Property code	Value	Unit	Source
gf	-226.46	kJ/mol	Joback Method
hf	-1260.61	kJ/mol	Joback Method
hfus	88.46	kJ/mol	Joback Method
hvap	111.43	kJ/mol	Joback Method
log10ws	-12.31		Crippen Method
logp	11.424		Crippen Method
mvol	518.890	ml/mol	McGowan Method
pc	498.69	kPa	Joback Method
rinpol	3490.00		NIST Webbook
rinpol	3490.00		NIST Webbook
tb	1152.34	K	Joback Method
tc	1512.06	K	Joback Method
tf	613.53	K	Joback Method
vc	2.038	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1935.25	J/molxK	1152.34	Joback Method
cpg	1963.71	J/molxK	1212.29	Joback Method
cpg	1987.73	J/molxK	1272.25	Joback Method
cpg	2007.68	J/molxK	1332.20	Joback Method
cpg	2023.92	J/molxK	1392.16	Joback Method
cpg	2036.81	J/molxK	1452.11	Joback Method
cpg	2046.70	J/molxK	1512.06	Joback Method
dvisc	0.0001284	Paxs	613.53	Joback Method

dvisc	0.0000516	Paxs	703.33	Joback Method
dvisc	0.0000255	Paxs	793.13	Joback Method
dvisc	0.0000145	Paxs	882.94	Joback Method
dvisc	0.0000092	Paxs	972.74	Joback Method
dvisc	0.0000063	Paxs	1062.54	Joback Method
dvisc	0.0000046	Paxs	1152.34	Joback Method

Sources

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=U416841&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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