

Sebacic acid, but-2-enyl heptadecyl ester

Inchi:	InChI=1S/C31H58O4/c1-3-5-7-8-9-10-11-12-13-14-15-16-19-22-25-29-35-31(33)27-24-2
InchiKey:	JVEUHNXHFJSG-GQCTYLIASA-N
Formula:	C31H58O4
SMILES:	CC=CCOC(=O)CCCCCCCC(=O)OCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]:	494.79

Physical Properties

Property code	Value	Unit	Source
gf	-177.48	kJ/mol	Joback Method
hf	-1055.55	kJ/mol	Joback Method
hfus	81.82	kJ/mol	Joback Method
hvap	102.87	kJ/mol	Joback Method
log10ws	-10.38		Crippen Method
logp	9.641		Crippen Method
mcvol	458.230	ml/mol	McGowan Method
pc	609.66	kPa	Joback Method
rinsol	3509.00		NIST Webbook
tb	1065.42	K	Joback Method
tc	1343.17	K	Joback Method
tf	578.37	K	Joback Method
vc	1.800	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1642.56	J/molxK	1065.42	Joback Method
cpg	1667.34	J/molxK	1111.71	Joback Method
cpg	1689.72	J/molxK	1158.00	Joback Method
cpg	1709.85	J/molxK	1204.29	Joback Method
cpg	1727.91	J/molxK	1250.59	Joback Method
cpg	1744.05	J/molxK	1296.88	Joback Method
cpg	1758.45	J/molxK	1343.17	Joback Method
dvisc	0.0001934	Paxs	578.37	Joback Method
dvisc	0.0000836	Paxs	659.54	Joback Method

dvisc	0.0000434	Paxs	740.72	Joback Method
dvisc	0.0000257	Paxs	821.89	Joback Method
dvisc	0.0000167	Paxs	903.07	Joback Method
dvisc	0.0000116	Paxs	984.25	Joback Method
dvisc	0.0000086	Paxs	1065.42	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=U356055&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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