Sebacic acid, hexadecyl 3-methylbut-3-enyl ester

Inchi: InChI=1S/C31H58O4/c1-4-5-6-7-8-9-10-11-12-13-14-17-20-23-27-34-30(32)24-21-18-15

InchiKey: AOXNRMPJXRUJCP-UHFFFAOYSA-N

Formula: C31H58O4

SMILES: C=C(C)CCOC(=O)CCCCCCCCC(=O)OCCCCCCCCCCCCCCCC

Mol. weight [g/mol]: 494.79

Physical Properties

Property code	Value	Unit	Source
gf	-178.41	kJ/mol	Joback Method
hf	-1057.13	kJ/mol	Joback Method
hfus	79.03	kJ/mol	Joback Method
hvap	102.32	kJ/mol	Joback Method
log10ws	-10.38		Crippen Method
logp	9.641		Crippen Method
mcvol	458.230	ml/mol	McGowan Method
pc	608.16	kPa	Joback Method
rinpol	3471.00		NIST Webbook
tb	1057.82	K	Joback Method
tc	1332.16	K	Joback Method
tf	567.73	K	Joback Method
vc	1.802	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1639.52	J/mol×K	1057.82	Joback Method
cpg	1663.86	J/mol×K	1103.54	Joback Method
cpg	1685.68	J/mol×K	1149.27	Joback Method
cpg	1705.12	J/mol×K	1194.99	Joback Method
cpg	1722.32	J/mol×K	1240.71	Joback Method
cpg	1737.43	J/mol×K	1286.43	Joback Method
cpg	1750.58	J/mol×K	1332.16	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=U355947&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
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