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

Inchi: InChI=1S/C30H56O4/c1-4-5-6-7-8-9-10-11-12-13-16-19-22-26-33-29(31)23-20-17-14-15

InchiKey: BXUARLAREHYKCG-UHFFFAOYSA-N

Formula: C30H56O4

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

Mol. weight [g/mol]: 480.76

Physical Properties

Property code	Value	Unit	Source
gf	-186.83	kJ/mol	Joback Method
hf	-1036.49	kJ/mol	Joback Method
hfus	76.44	kJ/mol	Joback Method
hvap	100.10	kJ/mol	Joback Method
log10ws	-9.96		Crippen Method
logp	9.251		Crippen Method
mcvol	444.140	ml/mol	McGowan Method
pc	638.01	kPa	Joback Method
rinpol	3360.00		NIST Webbook
tb	1034.94	K	Joback Method
tc	1294.63	K	Joback Method
tf	556.46	K	Joback Method
vc	1.746	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1574.01	J/mol×K	1034.94	Joback Method
cpg	1597.51	J/mol×K	1078.22	Joback Method
cpg	1618.73	J/mol×K	1121.50	Joback Method
cpg	1637.79	J/mol×K	1164.79	Joback Method
cpg	1654.81	J/mol×K	1208.07	Joback Method
cpg	1669.91	J/mol×K	1251.35	Joback Method
cpg	1683.20	J/mol×K	1294.63	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355946&Units=SI

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