Sebacic acid, hex-4-yn-3-yl pentadecyl ester

Inchi: InChI=1S/C31H56O4/c1-4-7-8-9-10-11-12-13-14-15-18-21-24-28-34-30(32)26-22-19-16-
InchiKey: IRRMVVIYSQHFAV-UHFFFAOYSA-N
Formula: C31H56O4
SMILES: CC#CC(CC)OC(=O)CCCCCCCCC(=O)OCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 492.77

Physical Properties

Property code	Value	Unit	Source
gf	-57.34	kJ/mol	Joback Method
hf	-905.75	kJ/mol	Joback Method
hfus	81.22	kJ/mol	Joback Method
hvap	104.68	kJ/mol	Joback Method
log10ws	-10.43		Crippen Method
logp	9.087		Crippen Method
mcvol	453.930	ml/mol	McGowan Method
pc	646.15	kPa	Joback Method
rinpol	3425.00		NIST Webbook
rinpol	3425.00		NIST Webbook
tb	1069.82	K	Joback Method
tc	1335.10	K	Joback Method
tf	674.55	K	Joback Method
vc	1.776	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1613.07	J/mol×K	1069.82	Joback Method
cpg	1635.10	J/mol×K	1114.03	Joback Method
cpg	1654.72	J/mol×K	1158.25	Joback Method
cpg	1672.03	J/mol×K	1202.46	Joback Method
cpg	1687.15	J/mol×K	1246.67	Joback Method
cpg	1700.17	J/mol×K	1290.88	Joback Method
cpg	1711.21	J/mol×K	1335.10	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=U355832&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

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