

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

Inchi:	InChI=1S/C30H54O4/c1-4-7-8-9-10-11-12-13-14-17-20-23-27-33-29(31)25-21-18-15-16-
InchiKey:	BFBBCICAZOZYNV-UHFFFAOYSA-N
Formula:	C30H54O4
SMILES:	CC#CC(CC)OC(=O)CCCCCCCCC(=O)OCCCCCCCCCCCCC
Mol. weight [g/mol]:	478.75

Physical Properties

Property code	Value	Unit	Source
gf	-65.76	kJ/mol	Joback Method
hf	-885.11	kJ/mol	Joback Method
hfus	78.63	kJ/mol	Joback Method
hvap	102.45	kJ/mol	Joback Method
log10ws	-10.01		Crippen Method
logp	8.697		Crippen Method
mvol	439.840	ml/mol	McGowan Method
pc	678.88	kPa	Joback Method
rinpol	3319.00		NIST Webbook
rinpol	3319.00		NIST Webbook
tb	1046.94	K	Joback Method
tc	1299.49	K	Joback Method
tf	663.28	K	Joback Method
vc	1.720	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1548.11	J/molxK	1046.94	Joback Method
cpg	1569.55	J/molxK	1089.03	Joback Method
cpg	1588.80	J/molxK	1131.12	Joback Method
cpg	1605.95	J/molxK	1173.21	Joback Method
cpg	1621.09	J/molxK	1215.31	Joback Method
cpg	1634.30	J/molxK	1257.40	Joback Method
cpg	1645.68	J/molxK	1299.49	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355831&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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