Sebacic acid, dodec-9-ynyl hexyl ester

Inchi: InChI=1S/C28H50O4/c1-3-5-7-9-10-11-12-15-18-22-26-32-28(30)24-20-17-14-13-16-19-
InchiKey: OEXURIGSDXIARG-UHFFFAOYSA-N
Formula: C28H50O4
SMILES: CCC#CCCCCCCCCOC(=O)CCCCCCCCC(=O)OCCCCCC
Mol. weight [g/mol]: 450.69

Physical Properties

Property code	Value	Unit	Source
gf	-80.16	kJ/mol	Joback Method
hf	-838.55	kJ/mol	Joback Method
hfus	76.97	kJ/mol	Joback Method
hvap	98.39	kJ/mol	Joback Method
log10ws	-9.06		Crippen Method
logp	7.918		Crippen Method
mcvol	411.660	ml/mol	McGowan Method
pc	748.97	kPa	Joback Method
rinpol	3226.00		NIST Webbook
rinpol	3226.00		NIST Webbook
tb	1001.62	K	Joback Method
tc	1234.79	K	Joback Method
tf	655.74	K	Joback Method
vc	1.613	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1418.69	J/mol×K	1001.62	Joback Method
cpg	1439.27	J/mol×K	1040.48	Joback Method
cpg	1458.03	J/mol×K	1079.34	Joback Method
cpg	1475.00	J/mol×K	1118.21	Joback Method
cpg	1490.27	J/mol×K	1157.07	Joback Method
cpg	1503.89	J/mol×K	1195.93	Joback Method
cpg	1515.92	J/mol×K	1234.79	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=U355793&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