Sebacic acid, dodec-9-ynyl heptyl ester

Inchi: InChI=1S/C29H52O4/c1-3-5-7-9-10-11-12-15-19-23-27-33-29(31)25-21-17-14-13-16-20-
InchiKey: ZSEOPPCOQRIJIR-UHFFFAOYSA-N
Formula: C29H52O4
SMILES: CCC#CCCCCCCCCOC(=O)CCCCCCCCC(=O)OCCCCCCC
Mol. weight [g/mol]: 464.72

Physical Properties

Property code	Value	Unit	Source
gf	-71.74	kJ/mol	Joback Method
hf	-859.19	kJ/mol	Joback Method
hfus	79.56	kJ/mol	Joback Method
hvap	100.61	kJ/mol	Joback Method
log10ws	-9.48		Crippen Method
logp	8.308		Crippen Method
mcvol	425.750	ml/mol	McGowan Method
pc	711.11	kPa	Joback Method
rinpol	3325.00		NIST Webbook
tb	1024.50	K	Joback Method
tc	1267.99	K	Joback Method
tf	667.01	K	Joback Method
vc	1.669	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1483.15	J/mol×K	1024.50	Joback Method
cpg	1504.29	J/mol×K	1065.08	Joback Method
cpg	1523.43	J/mol×K	1105.66	Joback Method
cpg	1540.62	J/mol×K	1146.25	Joback Method
cpg	1555.95	J/mol×K	1186.83	Joback Method
cpg	1569.50	J/mol×K	1227.41	Joback Method
cpg	1581.33	J/mol×K	1267.99	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=U355794&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