Sebacic acid, dodec-9-ynyl pentyl ester

Inchi: InChI=1S/C27H48O4/c1-3-5-7-8-9-10-11-14-17-21-25-31-27(29)23-19-16-13-12-15-18-2
InchiKey: OCHXVMKNWICFQG-UHFFFAOYSA-N
Formula: C27H48O4
SMILES: CCC#CCCCCCCCCOC(=O)CCCCCCCCC(=O)OCCCCC
Mol. weight [g/mol]: 436.67

Physical Properties

Property code	Value	Unit	Source
gf	-88.58	kJ/mol	Joback Method
hf	-817.91	kJ/mol	Joback Method
hfus	74.38	kJ/mol	Joback Method
hvap	96.16	kJ/mol	Joback Method
log10ws	-8.64		Crippen Method
logp	7.528		Crippen Method
mcvol	397.570	ml/mol	McGowan Method
pc	789.93	kPa	Joback Method
rinpol	3127.00		NIST Webbook
tb	978.74	K	Joback Method
tc	1202.90	K	Joback Method
tf	644.47	K	Joback Method
vc	1.558	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1354.57	J/mol×K	978.74	Joback Method
cpg	1374.64	J/mol×K	1016.10	Joback Method
cpg	1393.03	J/mol×K	1053.46	Joback Method
cpg	1409.79	J/mol×K	1090.82	Joback Method
cpg	1424.97	J/mol×K	1128.18	Joback Method
cpg	1438.62	J/mol×K	1165.54	Joback Method
cpg	1450.80	J/mol×K	1202.90	Joback Method

Sources

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=U355791&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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