Sebacic acid, propyl tridec-2-ynyl ester

Inchi: InChI=1S/C26H46O4/c1-3-5-6-7-8-9-10-11-14-17-20-24-30-26(28)22-19-16-13-12-15-18
InchiKey: CVVALNNFBXPSNZ-UHFFFAOYSA-N
Formula: C26H46O4
SMILES: CCCCCCCCCCC#CCOC(=O)CCCCCCCCC(=O)OCCC
Mol. weight [g/mol]: 422.64

Physical Properties

Property code	Value	Unit	Source
gf	-97.00	kJ/mol	Joback Method
hf	-797.27	kJ/mol	Joback Method
hfus	71.79	kJ/mol	Joback Method
hvap	93.93	kJ/mol	Joback Method
log10ws	-8.23		Crippen Method
logp	7.138		Crippen Method
mcvol	383.480	ml/mol	McGowan Method
pc	834.35	kPa	Joback Method
rinpol	3012.00		NIST Webbook
tb	955.86	K	Joback Method
tc	1172.24	K	Joback Method
tf	633.20	K	Joback Method
vc	1.502	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1290.85	J/mol×K	955.86	Joback Method
cpg	1310.44	J/mol×K	991.92	Joback Method
cpg	1328.48	J/mol×K	1027.99	Joback Method
cpg	1345.02	J/mol×K	1064.05	Joback Method
cpg	1360.10	J/mol×K	1100.11	Joback Method
cpg	1373.76	J/mol×K	1136.17	Joback Method
cpg	1386.04	J/mol×K	1172.24	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=U355855&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

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