Sebacic acid, heptyl tridec-2-ynyl ester

Inchi: InChI=1S/C30H54O4/c1-3-5-7-9-10-11-12-13-16-20-24-28-34-30(32)26-22-18-15-14-17-
InchiKey: KPPDNWJGGWFVCQ-UHFFFAOYSA-N
Formula: C30H54O4
SMILES: CCCCCCCCCCC#CCOC(=O)CCCCCCCCC(=O)OCCCCCCC
Mol. weight [g/mol]: 478.75

Physical Properties

Property code	Value	Unit	Source
gf	-63.32	kJ/mol	Joback Method
hf	-879.83	kJ/mol	Joback Method
hfus	82.15	kJ/mol	Joback Method
hvap	102.84	kJ/mol	Joback Method
log10ws	-9.90		Crippen Method
logp	8.698		Crippen Method
mcvol	439.840	ml/mol	McGowan Method
pc	676.05	kPa	Joback Method
rinpol	3412.00		NIST Webbook
tb	1047.38	K	Joback Method
tc	1302.61	K	Joback Method
tf	678.28	K	Joback Method
vc	1.726	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1547.91	J/mol×K	1047.38	Joback Method
cpg	1569.65	J/mol×K	1089.92	Joback Method
cpg	1589.18	J/mol×K	1132.46	Joback Method
cpg	1606.59	J/mol×K	1175.00	Joback Method
cpg	1621.96	J/mol×K	1217.54	Joback Method
cpg	1635.38	J/mol×K	1260.08	Joback Method
cpg	1646.96	J/mol×K	1302.61	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355861&Units=SI
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

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