Sebacic acid, di(non-5-yn-3-yl) ester

Inchi: InChI=1S/C28H46O4/c1-5-9-11-17-21-25(7-3)31-27(29)23-19-15-13-14-16-20-24-28(30)32-26(8-4)22-18-12-10-6-2/h25-26H,5-6,9-14,19-24H2,1-4,7-8H3
InchiKey: HLAOCHLEWZVYHZ-UHFFFAOYSA-N
Formula: C28H46O4
SMILES: CCCC#CCC(CC)OC(=O)CCCCCCCCC(=O)OC(CC)CC#CCCC
Mol. weight [g/mol]: 446.66

Physical Properties

Property code	Value	Unit	Source
gf	117.76	kJ/mol	Joback Method
hf	-576.81	kJ/mol	Joback Method
hfus	73.05	kJ/mol	Joback Method
hvap	99.76	kJ/mol	Joback Method
log10ws	-9.08		Crippen Method
logp	7.138		Crippen Method
mcvol	403.060	ml/mol	McGowan Method
pc	826.69	kPa	Joback Method
rinpol	3017.00		NIST Webbook
tb	1009.74	K	Joback Method
tc	1237.28	K	Joback Method
tf	731.84	K	Joback Method
vc	1.563	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1362.79	J/mol×K	1009.74	Joback Method
cpg	1381.32	J/mol×K	1047.66	Joback Method
cpg	1398.17	J/mol×K	1085.59	Joback Method
cpg	1413.38	J/mol×K	1123.51	Joback Method
cpg	1427.01	J/mol×K	1161.44	Joback Method
cpg	1439.09	J/mol×K	1199.36	Joback Method
cpg	1449.68	J/mol×K	1237.28	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=U355803&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