Sebacic acid, 2-methyloct-5-yn-4-yl propyl ester

Inchi: InChI=1S/C22H38O4/c1-5-7-14-20(18-19(3)4)26-22(24)16-13-11-9-8-10-12-15-21(23)25
InchiKey: IENDVDYWTHIQQX-UHFFFAOYSA-N
Formula: C22H38O4
SMILES: CCC#CC(CC(C)C)OC(=O)CCCCCCCCC(=O)OCCC
Mol. weight [g/mol]: 366.53

Physical Properties

Property code	Value	Unit	Source
gf	-135.56	kJ/mol	Joback Method
hf	-725.27	kJ/mol	Joback Method
hfus	54.39	kJ/mol	Joback Method
hvap	84.25	kJ/mol	Joback Method
log10ws	-6.42		Crippen Method
logp	5.432		Crippen Method
mcvol	327.120	ml/mol	McGowan Method
pc	1066.57	kPa	Joback Method
rinpol	2420.00		NIST Webbook
tb	863.46	K	Joback Method
tc	1060.75	K	Joback Method
tf	558.12	K	Joback Method
vc	1.266	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1041.86	J/mol×K	863.46	Joback Method
cpg	1059.98	J/mol×K	896.34	Joback Method
cpg	1076.90	J/mol×K	929.22	Joback Method
cpg	1092.63	J/mol×K	962.11	Joback Method
cpg	1107.20	J/mol×K	994.99	Joback Method
cpg	1120.63	J/mol×K	1027.87	Joback Method
cpg	1132.95	J/mol×K	1060.75	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355867&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