Sebacic acid, heptyl neopentyl ester

Inchi: InChI=1S/C22H42O4/c1-5-6-7-12-15-18-25-20(23)16-13-10-8-9-11-14-17-21(24)26-19-2
InchiKey: DQKAYUGBQBLMAS-UHFFFAOYSA-N
Formula: C22H42O4
SMILES: CCCCCCCOC(=O)CCCCCCCCC(=O)OCC(C)(C)C
Mol. weight [g/mol]: 370.57

Physical Properties

Property code	Value	Unit	Source
gf	-330.64	kJ/mol	Joback Method
hf	-995.76	kJ/mol	Joback Method
hfus	50.90	kJ/mol	Joback Method
hvap	81.58	kJ/mol	Joback Method
log10ws	-6.51		Crippen Method
logp	6.210		Crippen Method
mcvol	335.720	ml/mol	McGowan Method
pc	965.07	kPa	Joback Method
rinpol	2520.00		NIST Webbook
tb	852.11	K	Joback Method
tc	1044.11	K	Joback Method
tf	484.44	K	Joback Method
vc	1.304	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1092.56	J/mol×K	852.11	Joback Method
cpg	1111.54	J/mol×K	884.11	Joback Method
cpg	1129.36	J/mol×K	916.11	Joback Method
cpg	1146.06	J/mol×K	948.11	Joback Method
cpg	1161.66	J/mol×K	980.11	Joback Method
cpg	1176.22	J/mol×K	1012.11	Joback Method
cpg	1189.77	J/mol×K	1044.11	Joback Method
dvisc	0.0006242	Pa×s	484.44	Joback Method
dvisc	0.0002865	Pa×s	545.72	Joback Method

dvisc	0.0001539	Pa×s	607.00	Joback Method
dvisc	0.0000927	Pa×s	668.27	Joback Method
dvisc	0.0000608	Pa×s	729.55	Joback Method
dvisc	0.0000425	Pa×s	790.83	Joback Method
dvisc	0.0000313	Pa×s	852.11	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=U354468&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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