Sebacic acid, hexyl 3-methylpentyl ester

Inchi: InChI=1S/C22H42O4/c1-4-6-7-14-18-25-21(23)15-12-10-8-9-11-13-16-22(24)26-19-17-2
InchiKey: OQZNLCIOUFXJJZ-UHFFFAOYSA-N
Formula: C22H42O4
SMILES: CCCCCCOC(=O)CCCCCCCCC(=O)OCCC(C)CC
Mol. weight [g/mol]: 370.57

Physical Properties

Property code	Value	Unit	Source
gf	-335.92	kJ/mol	Joback Method
hf	-992.29	kJ/mol	Joback Method
hfus	54.79	kJ/mol	Joback Method
hvap	82.49	kJ/mol	Joback Method
log10ws	-6.51		Crippen Method
logp	6.210		Crippen Method
mcvol	335.720	ml/mol	McGowan Method
pc	958.51	kPa	Joback Method
rinpol	2526.00		NIST Webbook
tb	854.90	K	Joback Method
tc	1046.82	K	Joback Method
tf	467.02	K	Joback Method
vc	1.310	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1092.52	J/mol×K	854.90	Joback Method
cpg	1111.68	J/mol×K	886.89	Joback Method
cpg	1129.63	J/mol×K	918.87	Joback Method
cpg	1146.40	J/mol×K	950.86	Joback Method
cpg	1162.01	J/mol×K	982.84	Joback Method
cpg	1176.47	J/mol×K	1014.83	Joback Method
cpg	1189.83	J/mol×K	1046.82	Joback Method
dvisc	0.0007814	Pa×s	467.02	Joback Method
dvisc	0.0003435	Pa×s	531.67	Joback Method

dvisc	0.0001805	Pa×s	596.31	Joback Method
dvisc	0.0001075	Pa×s	660.96	Joback Method
dvisc	0.0000703	Pa×s	725.61	Joback Method
dvisc	0.0000492	Pa×s	790.25	Joback Method
dvisc	0.0000364	Pa×s	854.90	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=U355617&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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