Sebacic acid, 3,3-dimethylbut-2-yl hexyl ester

Inchi: InChI=1S/C22H42O4/c1-6-7-8-15-18-25-20(23)16-13-11-9-10-12-14-17-21(24)26-19(2)22(3,4)5

InchiKey: RMDMVFUKCSPOBW-UHFFFAOYSA-N

Formula: C22H42O4

SMILES: CCCCCCOC(=O)CCCCCCCCC(=O)OC(C)C(C)(C)C

Mol. weight [g/mol]: 370.57

Physical Properties

Property code	Value	Unit	Source
gf	-333.08	kJ/mol	Joback Method
hf	-1001.04	kJ/mol	Joback Method
hfus	47.37	kJ/mol	Joback Method
hvap	81.19	kJ/mol	Joback Method
log10ws	-6.63		Crippen Method
logp	6.209		Crippen Method
mcvol	335.720	ml/mol	McGowan Method
pc	969.88	kPa	Joback Method
rinpol	2455.00		NIST Webbook
rinpol	2455.00		NIST Webbook
tb	851.67	K	Joback Method
tc	1044.13	K	Joback Method
tf	469.44	K	Joback Method
vc	1.298	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1093.02	J/mol×K	851.67	Joback Method
cpg	1176.71	J/mol×K	1012.05	Joback Method
cpg	1162.18	J/mol×K	979.97	Joback Method
cpg	1146.58	J/mol×K	947.90	Joback Method
cpg	1129.88	J/mol×K	915.82	Joback Method
cpg	1112.04	J/mol×K	883.75	Joback Method
cpg	1190.22	J/mol×K	1044.13	Joback Method
dvisc	0.0000287	Pa×s	851.67	Joback Method

dvisc	0.0000396	Pa×s	787.97	Joback Method
dvisc	0.0000579	Pa×s	724.26	Joback Method
dvisc	0.0000910	Pa×s	660.56	Joback Method
dvisc	0.0001576	Pa×s	596.85	Joback Method
dvisc	0.0003111	Pa×s	533.14	Joback Method
dvisc	0.0007385	Pa×s	469.44	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=U355600&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