Sebacic acid, isobutyl oct-3-yl ester

Inchi: InChI=1S/C22H42O4/c1-5-7-12-15-20(6-2)26-22(24)17-14-11-9-8-10-13-16-21(23)25-18
InchiKey: LTFRTPCNJDUBQY-UHFFFAOYSA-N
Formula: C22H42O4
SMILES: CCCCCC(CC)OC(=O)CCCCCCCCC(=O)OCC(C)C
Mol. weight [g/mol]: 370.57

Physical Properties

Property code	Value	Unit	Source
gf	-338.36	kJ/mol	Joback Method
hf	-997.57	kJ/mol	Joback Method
hfus	51.26	kJ/mol	Joback Method
hvap	82.10	kJ/mol	Joback Method
log10ws	-6.63		Crippen Method
logp	6.209		Crippen Method
mcvol	335.720	ml/mol	McGowan Method
pc	963.27	kPa	Joback Method
rinpol	2337.00		NIST Webbook
rinpol	2337.00		NIST Webbook
tb	854.46	K	Joback Method
tc	1046.57	K	Joback Method
tf	452.02	K	Joback Method
vc	1.304	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1092.98	J/mol×K	854.46	Joback Method
cpg	1112.15	J/mol×K	886.48	Joback Method
cpg	1130.10	J/mol×K	918.50	Joback Method
cpg	1146.85	J/mol×K	950.51	Joback Method
cpg	1162.43	J/mol×K	982.53	Joback Method
cpg	1176.86	J/mol×K	1014.55	Joback Method
cpg	1190.16	J/mol×K	1046.57	Joback Method
dvisc	0.0009298	Pa×s	452.02	Joback Method

dvisc	0.0003731	Pa×s	519.09	Joback Method
dvisc	0.0001845	Pa×s	586.17	Joback Method
dvisc	0.0001055	Pa×s	653.24	Joback Method
dvisc	0.0000669	Pa×s	720.31	Joback Method
dvisc	0.0000458	Pa×s	787.39	Joback Method
dvisc	0.0000333	Pa×s	854.46	Joback Method

Sources

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=U416827&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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