

Sebacic acid, 3-hexyl isoheptyl ester

Inchi:	InChI=1S/C22H42O4/c1-5-14-20(6-2)26-22(24)17-12-10-8-7-9-11-16-21(23)25-18-13-15
InchiKey:	RXLGAGZIIYJGPOT-UHFFFAOYSA-N
Formula:	C22H42O4
SMILES:	CCCC(CC)OC(=O)CCCCCCCC(=O)OCCCC(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
mvol	335.720	ml/mol	McGowan Method
pc	963.27	kPa	Joback Method
rinpol	2453.00		NIST Webbook
rinpol	2453.00		NIST Webbook
tb	854.46	K	Joback Method
tc	1046.57	K	Joback Method
tf	452.02	K	Joback Method
vc	1.304	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1092.98	J/molxK	854.46	Joback Method
cpg	1176.86	J/molxK	1014.55	Joback Method
cpg	1162.43	J/molxK	982.53	Joback Method
cpg	1146.85	J/molxK	950.51	Joback Method
cpg	1130.10	J/molxK	918.50	Joback Method
cpg	1112.15	J/molxK	886.48	Joback Method
cpg	1190.16	J/molxK	1046.57	Joback Method
dvisc	0.0000333	Paxs	854.46	Joback Method

dvisc	0.0000458	Paxs	787.39	Joback Method
dvisc	0.0000669	Paxs	720.31	Joback Method
dvisc	0.0001055	Paxs	653.24	Joback Method
dvisc	0.0001845	Paxs	586.17	Joback Method
dvisc	0.0003731	Paxs	519.09	Joback Method
dvisc	0.0009298	Paxs	452.02	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355540&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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