

Sebacic acid, 3-heptyl isoheptyl ester

Inchi:	InChI=1S/C23H44O4/c1-5-7-16-21(6-2)27-23(25)18-13-11-9-8-10-12-17-22(24)26-19-14
InchiKey:	XQQPXBWQYTSOJ-UHFFFAOYSA-N
Formula:	C23H44O4
SMILES:	CCCCC(CC)OC(=O)CCCCCCCCC(=O)OCCCC(C)C
Mol. weight [g/mol]:	384.59

Physical Properties

Property code	Value	Unit	Source
gf	-329.94	kJ/mol	Joback Method
hf	-1018.21	kJ/mol	Joback Method
hfus	53.85	kJ/mol	Joback Method
hvap	84.33	kJ/mol	Joback Method
log10ws	-7.05		Crippen Method
logp	6.599		Crippen Method
mvol	349.810	ml/mol	McGowan Method
pc	908.34	kPa	Joback Method
rinpol	2541.00		NIST Webbook
tb	877.34	K	Joback Method
tc	1074.11	K	Joback Method
tf	463.29	K	Joback Method
vc	1.359	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1155.40	J/molxK	877.34	Joback Method
cpg	1174.99	J/molxK	910.14	Joback Method
cpg	1193.27	J/molxK	942.93	Joback Method
cpg	1210.26	J/molxK	975.73	Joback Method
cpg	1226.01	J/molxK	1008.52	Joback Method
cpg	1240.52	J/molxK	1041.32	Joback Method
cpg	1253.84	J/molxK	1074.11	Joback Method
dvisc	0.0008160	Paxs	463.29	Joback Method
dvisc	0.0003252	Paxs	532.30	Joback Method

dvisc	0.0001600	Paxs	601.31	Joback Method
dvisc	0.0000911	Paxs	670.32	Joback Method
dvisc	0.0000577	Paxs	739.32	Joback Method
dvisc	0.0000394	Paxs	808.33	Joback Method
dvisc	0.0000286	Paxs	877.34	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355579&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

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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