

Sebacic acid, 8-chlorooctyl isohexyl ester

Inchi:	InChI=1S/C24H45ClO4/c1-22(2)16-15-21-29-24(27)18-12-8-4-3-7-11-17-23(26)28-20-14
InchiKey:	VUYIZNIWHUIJKF-UHFFFAOYSA-N
Formula:	C24H45ClO4
SMILES:	CC(C)CCCOC(=O)CCCCCCCCC(=O)OCCCCCCCCCI
Mol. weight [g/mol]:	433.06

Physical Properties

Property code	Value	Unit	Source
gf	-331.01	kJ/mol	Joback Method
hf	-1049.31	kJ/mol	Joback Method
hfus	64.16	kJ/mol	Joback Method
hvap	91.33	kJ/mol	Joback Method
log10ws	-7.51		Crippen Method
logp	7.209		Crippen Method
mcvol	376.140	ml/mol	McGowan Method
pc	835.79	kPa	Joback Method
rinsol	3068.00		NIST Webbook
tb	938.09	K	Joback Method
tc	1150.89	K	Joback Method
tf	519.48	K	Joback Method
vc	1.470	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1248.90	J/molxK	938.09	Joback Method
cpg	1268.05	J/molxK	973.56	Joback Method
cpg	1285.71	J/molxK	1009.02	Joback Method
cpg	1301.93	J/molxK	1044.49	Joback Method
cpg	1316.73	J/molxK	1079.96	Joback Method
cpg	1330.17	J/molxK	1115.42	Joback Method
cpg	1342.28	J/molxK	1150.89	Joback Method
dvisc	0.0004616	Paxs	519.48	Joback Method
dvisc	0.0002071	Paxs	589.25	Joback Method

dvisc	0.0001101	Paxs	659.02	Joback Method
dvisc	0.0000661	Paxs	728.79	Joback Method
dvisc	0.0000434	Paxs	798.55	Joback Method
dvisc	0.0000304	Paxs	868.32	Joback Method
dvisc	0.0000225	Paxs	938.09	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355532&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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