

Fumaric acid, 8-chlorooctyl isohexyl ester

Inchi:	InChI=1S/C18H31ClO4/c1-16(2)10-9-15-23-18(21)12-11-17(20)22-14-8-6-4-3-5-7-13-19
InchiKey:	NBCAIVJHQAZWID-VAWYXSNFSA-N
Formula:	C18H31ClO4
SMILES:	CC(C)CCCOC(=O)C=CC(=O)OCCCCCCCCCI
Mol. weight [g/mol]:	346.89

Physical Properties

Property code	Value	Unit	Source
gf	-301.31	kJ/mol	Joback Method
hf	-808.25	kJ/mol	Joback Method
hfus	48.83	kJ/mol	Joback Method
hvap	77.93	kJ/mol	Joback Method
log10ws	-4.85		Crippen Method
logp	4.645		Crippen Method
mcvol	287.300	ml/mol	McGowan Method
pc	1247.73	kPa	Joback Method
rinsol	2461.00		NIST Webbook
tb	804.97	K	Joback Method
tc	994.12	K	Joback Method
tf	446.78	K	Joback Method
vc	1.115	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	856.22	J/molxK	804.97	Joback Method
cpg	927.52	J/molxK	962.59	Joback Method
cpg	915.05	J/molxK	931.07	Joback Method
cpg	901.70	J/molxK	899.54	Joback Method
cpg	887.47	J/molxK	868.02	Joback Method
cpg	872.31	J/molxK	836.49	Joback Method
cpg	939.15	J/molxK	994.12	Joback Method
dvisc	0.0000489	Paxs	804.97	Joback Method
dvisc	0.0000654	Paxs	745.27	Joback Method

dvisc	0.0000920	Paxs	685.57	Joback Method
dvisc	0.0001383	Paxs	625.88	Joback Method
dvisc	0.0002265	Paxs	566.18	Joback Method
dvisc	0.0004166	Paxs	506.48	Joback Method
dvisc	0.0009018	Paxs	446.78	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348532&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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