

Fumaric acid, 8-chlorooctyl hexyl ester

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

Physical Properties

Property code	Value	Unit	Source
gf	-298.87	kJ/mol	Joback Method
hf	-802.97	kJ/mol	Joback Method
hfus	52.35	kJ/mol	Joback Method
hvap	78.32	kJ/mol	Joback Method
log10ws	-5.09		Crippen Method
logp	4.789		Crippen Method
mcvol	287.300	ml/mol	McGowan Method
pc	1240.71	kPa	Joback Method
rinsol	2505.00		NIST Webbook
tb	805.41	K	Joback Method
tc	993.22	K	Joback Method
tf	461.78	K	Joback Method
vc	1.121	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	855.70	J/mol×K	805.41	Joback Method
cpg	871.68	J/mol×K	836.71	Joback Method
cpg	886.75	J/mol×K	868.01	Joback Method
cpg	900.91	J/mol×K	899.31	Joback Method
cpg	914.21	J/mol×K	930.62	Joback Method
cpg	926.66	J/mol×K	961.92	Joback Method
cpg	938.28	J/mol×K	993.22	Joback Method
dvisc	0.0007679	Paxs	461.78	Joback Method
dvisc	0.0003850	Paxs	519.05	Joback Method

dvisc	0.0002214	Paxs	576.32	Joback Method
dvisc	0.0001407	Paxs	633.60	Joback Method
dvisc	0.0000964	Paxs	690.87	Joback Method
dvisc	0.0000700	Paxs	748.14	Joback Method
dvisc	0.0000532	Paxs	805.41	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348533&Units=SI

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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