Fumaric acid, 8-chlorooctyl isobutyl ester

Inchi: InChI=1S/C16H27ClO4/c1-14(2)13-21-16(19)10-9-15(18)20-12-8-6-4-3-5-7-11-17/h9-10,
InchiKey: MRHRYQMLUYULBY-MDZDMXLPSA-N
Formula: C16H27ClO4
SMILES: CC(C)COC(=O)C=CC(=O)OCCCCCCCCCl
Mol. weight [g/mol]: 318.84

Physical Properties

Property code	Value	Unit	Source
gf	-318.15	kJ/mol	Joback Method
hf	-766.97	kJ/mol	Joback Method
hfus	43.65	kJ/mol	Joback Method
hvap	73.48	kJ/mol	Joback Method
log10ws	-4.01		Crippen Method
logp	3.864		Crippen Method
mcvol	259.120	ml/mol	McGowan Method
pc	1435.89	kPa	Joback Method
rinpol	2249.00		NIST Webbook
rinpol	2249.00		NIST Webbook
tb	759.21	K	Joback Method
tc	946.71	K	Joback Method
tf	424.24	K	Joback Method
vc	1.002	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	740.99	J/mol×K	759.21	Joback Method
cpg	809.35	J/mol×K	915.46	Joback Method
cpg	797.32	J/mol×K	884.21	Joback Method
cpg	784.49	J/mol×K	852.96	Joback Method
cpg	770.83	J/mol×K	821.71	Joback Method
cpg	756.34	J/mol×K	790.46	Joback Method
cpg	820.60	J/mol×K	946.71	Joback Method
dvisc	0.0000650	Pa×s	759.21	Joback Method

dvisc	0.0000865	Pa×s	703.38	Joback Method
dvisc	0.0001210	Pa×s	647.55	Joback Method
dvisc	0.0001804	Pa×s	591.72	Joback Method
dvisc	0.0002921	Pa×s	535.90	Joback Method
dvisc	0.0005293	Pa×s	480.07	Joback Method
dvisc	0.0011214	Pa×s	424.24	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U348529&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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