Fumaric acid, 10-chlorodecyl ethyl ester

Inchi: InChI=1S/C16H27ClO4/c1-2-20-15(18)11-12-16(19)21-14-10-8-6-4-3-5-7-9-13-17/h11-12
InchiKey: YWJKCIKKRUGLIM-VAWYXSNFSA-N
Formula: C16H27ClO4
SMILES: CCOC(=O)C=CC(=O)OCCCCCCCCCCCCl
Mol. weight [g/mol]: 318.84

Physical Properties

Property code	Value	Unit	Source
gf	-315.71	kJ/mol	Joback Method
hf	-761.69	kJ/mol	Joback Method
hfus	47.17	kJ/mol	Joback Method
hvap	73.86	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	4.008		Crippen Method
mcvol	259.120	ml/mol	McGowan Method
pc	1427.22	kPa	Joback Method
rinpol	2294.00		NIST Webbook
rinpol	2294.00		NIST Webbook
tb	759.65	K	Joback Method
tc	945.22	K	Joback Method
tf	439.24	K	Joback Method
vc	1.008	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	740.46	J/mol×K	759.65	Joback Method
cpg	755.65	J/mol×K	790.58	Joback Method
cpg	770.00	J/mol×K	821.51	Joback Method
cpg	783.54	J/mol×K	852.44	Joback Method
cpg	796.28	J/mol×K	883.37	Joback Method
cpg	808.24	J/mol×K	914.29	Joback Method
cpg	819.45	J/mol×K	945.22	Joback Method
dvisc	0.0009436	Pa×s	439.24	Joback Method

dvisc	0.0004845	Pa×s	492.64	Joback Method
dvisc	0.0002834	Pa×s	546.04	Joback Method
dvisc	0.0001824	Pa×s	599.44	Joback Method
dvisc	0.0001262	Pa×s	652.85	Joback Method
dvisc	0.0000923	Pa×s	706.25	Joback Method
dvisc	0.0000705	Pa×s	759.65	Joback Method

Sources

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=U348305&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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