Fumaric acid, 8-chlorooctyl pentyl ester

Inchi: InChI=1S/C17H29ClO4/c1-2-3-9-14-21-16(19)11-12-17(20)22-15-10-7-5-4-6-8-13-18/h11
InchiKey: YQMHYKJAOJMLTC-VAWYXSNFSA-N
Formula: C17H29ClO4
SMILES: CCCCCOC(=O)C=CC(=O)OCCCCCCCCCl
Mol. weight [g/mol]: 332.86

Physical Properties

Property code	Value	Unit	Source
gf	-307.29	kJ/mol	Joback Method
hf	-782.33	kJ/mol	Joback Method
hfus	49.76	kJ/mol	Joback Method
hvap	76.09	kJ/mol	Joback Method
log10ws	-4.67		Crippen Method
logp	4.399		Crippen Method
mcvol	273.210	ml/mol	McGowan Method
pc	1329.07	kPa	Joback Method
rinpol	2402.00		NIST Webbook
rinpol	2402.00		NIST Webbook
tb	782.53	K	Joback Method
tc	968.90	K	Joback Method
tf	450.51	K	Joback Method
vc	1.065	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	797.60	J/mol×K	782.53	Joback Method
cpg	813.19	J/mol×K	813.59	Joback Method
cpg	827.90	J/mol×K	844.65	Joback Method
cpg	841.76	J/mol×K	875.72	Joback Method
cpg	854.78	J/mol×K	906.78	Joback Method
cpg	867.00	J/mol×K	937.84	Joback Method
cpg	878.43	J/mol×K	968.90	Joback Method
dvisc	0.0008532	Pa×s	450.51	Joback Method

dvisc	0.0004328	Pa×s	505.85	Joback Method
dvisc	0.0002510	Pa×s	561.18	Joback Method
dvisc	0.0001605	Pa×s	616.52	Joback Method
dvisc	0.0001105	Pa×s	671.86	Joback Method
dvisc	0.0000805	Pa×s	727.19	Joback Method
dvisc	0.0000613	Pa×s	782.53	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=U348531&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