Fumaric acid, 8-chlorooctyl heptyl ester

Inchi: InChI=1S/C19H33ClO4/c1-2-3-4-8-11-16-23-18(21)13-14-19(22)24-17-12-9-6-5-7-10-15-
InchiKey: FBIIAROAPWHMQC-BUHFOSPRSA-N
Formula: C19H33ClO4
SMILES: CCCCCCCOC(=O)C=CC(=O)OCCCCCCCCCl
Mol. weight [g/mol]: 360.92

Physical Properties

Property code	Value	Unit	Source
gf	-290.45	kJ/mol	Joback Method
hf	-823.61	kJ/mol	Joback Method
hfus	54.94	kJ/mol	Joback Method
hvap	80.54	kJ/mol	Joback Method
log10ws	-5.51		Crippen Method
logp	5.179		Crippen Method
mcvol	301.390	ml/mol	McGowan Method
pc	1160.87	kPa	Joback Method
rinpol	2608.00		NIST Webbook
rinpol	2608.00		NIST Webbook
tb	828.29	K	Joback Method
tc	1018.24	K	Joback Method
tf	473.05	K	Joback Method
vc	1.177	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	914.69	J/mol×K	828.29	Joback Method
cpg	931.08	J/mol×K	859.95	Joback Method
cpg	946.49	J/mol×K	891.61	Joback Method
cpg	960.96	J/mol×K	923.26	Joback Method
cpg	974.51	J/mol×K	954.92	Joback Method
cpg	987.18	J/mol×K	986.58	Joback Method
cpg	998.98	J/mol×K	1018.24	Joback Method
dvisc	0.0006884	Pa×s	473.05	Joback Method

dvisc	0.0003413	Pa×s	532.26	Joback Method
dvisc	0.0001947	Pa×s	591.46	Joback Method
dvisc	0.0001231	Pa×s	650.67	Joback Method
dvisc	0.0000839	Pa×s	709.88	Joback Method
dvisc	0.0000607	Pa×s	769.08	Joback Method
dvisc	0.0000460	Pa×s	828.29	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348534&Units=SI
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

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