Fumaric acid, 2-pentyl 8-chlorooctyl ester

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

Physical Properties

Property code	Value	Unit	Source
gf	-309.73	kJ/mol	Joback Method
hf	-787.61	kJ/mol	Joback Method
hfus	46.24	kJ/mol	Joback Method
hvap	75.70	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	4.397		Crippen Method
mcvol	273.210	ml/mol	McGowan Method
pc	1336.86	kPa	Joback Method
rinpol	2309.00		NIST Webbook
rinpol	2309.00		NIST Webbook
tb	782.09	K	Joback Method
tc	970.10	K	Joback Method
tf	435.51	K	Joback Method
vc	1.058	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	798.12	J/mol×K	782.09	Joback Method
cpg	867.99	J/mol×K	938.76	Joback Method
cpg	855.73	J/mol×K	907.43	Joback Method
cpg	842.63	J/mol×K	876.09	Joback Method
cpg	828.68	J/mol×K	844.76	Joback Method
cpg	813.85	J/mol×K	813.42	Joback Method
cpg	879.45	J/mol×K	970.10	Joback Method
dvisc	0.0000564	Pa×s	782.09	Joback Method

dvisc	0.0000753	Pa×s	724.33	Joback Method
dvisc	0.0001057	Pa×s	666.56	Joback Method
dvisc	0.0001582	Pa×s	608.80	Joback Method
dvisc	0.0002577	Pa×s	551.04	Joback Method
dvisc	0.0004705	Pa×s	493.27	Joback Method
dvisc	0.0010078	Pa×s	435.51	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405565&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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