Fumaric acid, pentafluorobenzyl 8-chlorooctyl ester

Inchi: InChI=1S/C19H20ClF5O4/c20-9-5-3-1-2-4-6-10-28-13(26)7-8-14(27)29-11-12-15(21)17(2

InchiKey: MVLMMLFTGSPJTM-BQYQJAHWSA-N

Formula: C19H20ClF5O4

SMILES: O=C(C=CC(=O)OCc1c(F)c(F)c(F)c(F)c1F)OCCCCCCCCCCl

Mol. weight [g/mol]: 442.81

Physical Properties

Property code	Value	Unit	Source
gf	-1200.24	kJ/mol	Joback Method
hf	-1624.98	kJ/mol	Joback Method
hfus	62.43	kJ/mol	Joback Method
hvap	82.04	kJ/mol	Joback Method
log10ws	-6.76		Crippen Method
logp	5.104		Crippen Method
mcvol	286.480	ml/mol	McGowan Method
pc	1185.79	kPa	Joback Method
rinpol	2550.00		NIST Webbook
tb	876.22	K	Joback Method
tc	1073.57	K	Joback Method
tf	565.02	K	Joback Method
vc	1.159	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	851.71	J/mol×K	876.22	Joback Method
cpg	864.21	J/mol×K	909.11	Joback Method
cpg	875.77	J/mol×K	942.00	Joback Method
cpg	886.41	J/mol×K	974.90	Joback Method
cpg	896.13	J/mol×K	1007.79	Joback Method
cpg	904.96	J/mol×K	1040.68	Joback Method
cpg	912.92	J/mol×K	1073.57	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=U405885&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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