Fumaric acid, 4-chlorobenzyl 2,2,3,3-tetrafluoropropyl ester

Inchi: InChI=1S/C14H11ClF4O4/c15-10-3-1-9(2-4-10)7-22-11(20)5-6-12(21)23-8-14(18,19)13(1

InchiKey: ADUNIUYHDAWPBS-AATRIKPKSA-N

Formula: C14H11ClF4O4

SMILES: O=C(C=CC(=O)OCC(F)(F)C(F)F)OCc1ccc(Cl)cc1

Mol. weight [g/mol]: 354.68

Physical Properties

Property code	Value	Unit	Source
gf	-1008.61	kJ/mol	Joback Method
hf	-1293.82	kJ/mol	Joback Method
hfus	37.02	kJ/mol	Joback Method
hvap	67.40	kJ/mol	Joback Method
log10ws	-4.17		Crippen Method
logp	3.383		Crippen Method
mcvol	214.260	ml/mol	McGowan Method
pc	1903.58	kPa	Joback Method
rinpol	1942.00		NIST Webbook
tb	738.96	K	Joback Method
tc	937.84	K	Joback Method
tf	445.42	K	Joback Method
vc	0.844	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	575.85	J/mol×K	738.96	Joback Method
cpg	586.95	J/mol×K	772.11	Joback Method
cpg	597.22	J/mol×K	805.25	Joback Method
cpg	606.71	J/mol×K	838.40	Joback Method
cpg	615.46	J/mol×K	871.55	Joback Method
cpg	623.50	J/mol×K	904.69	Joback Method
cpg	630.88	J/mol×K	937.84	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=U405912&Units=SI

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