Fumaric acid, 4-chlorobenzyl 2,2,3,3,4,4,5,5-octafluoropentyl ester

Inchi: InChI=1S/C16H11ClF8O4/c17-10-3-1-9(2-4-10)7-28-11(26)5-6-12(27)29-8-14(20,21)16(

InchiKey: VDQBIVORUJXYSW-AATRIKPKSA-N

Formula: C16H11ClF8O4

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

Mol. weight [g/mol]: 454.70

Physical Properties

Property code	Value	Unit	Source
gf	-1765.33	kJ/mol	Joback Method
hf	-2137.04	kJ/mol	Joback Method
hfus	39.70	kJ/mol	Joback Method
hvap	65.99	kJ/mol	Joback Method
log10ws	-5.64		Crippen Method
logp	4.654		Crippen Method
mcvol	249.520	ml/mol	McGowan Method
pc	1450.14	kPa	Joback Method
rinpol	2046.00		NIST Webbook
rinpol	2046.00		NIST Webbook
tb	775.34	K	Joback Method
tc	964.07	K	Joback Method
tf	475.16	K	Joback Method
vc	1.006	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	717.73	J/mol×K	775.34	Joback Method
cpg	728.24	J/mol×K	806.79	Joback Method
cpg	737.94	J/mol×K	838.25	Joback Method
cpg	746.88	J/mol×K	869.70	Joback Method
cpg	755.14	J/mol×K	901.16	Joback Method
cpg	762.80	J/mol×K	932.61	Joback Method
cpg	769.91	J/mol×K	964.07	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=U405913&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