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

Inchi: InChI=1S/C17H15ClF8O4/c18-11-6-4-10(5-7-11)8-29-12(27)2-1-3-13(28)30-9-15(21,22)1

InchiKey: BXCIWERIMYAROW-UHFFFAOYSA-N

Formula: C17H15ClF8O4

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

Mol. weight [g/mol]: 470.74

Physical Properties

Property code	Value	Unit	Source
gf	-1837.13	kJ/mol	Joback Method
hf	-2274.90	kJ/mol	Joback Method
hfus	42.08	kJ/mol	Joback Method
hvap	68.26	kJ/mol	Joback Method
log10ws	-6.20		Crippen Method
logp	5.268		Crippen Method
mcvol	267.910	ml/mol	McGowan Method
pc	1299.53	kPa	Joback Method
rinpol	2128.00		NIST Webbook
rinpol	2128.00		NIST Webbook
tb	794.06	K	Joback Method
tc	980.06	K	Joback Method
tf	491.51	K	Joback Method
vc	1.081	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	797.68	J/mol×K	794.06	Joback Method
cpg	809.19	J/mol×K	825.06	Joback Method
cpg	819.84	J/mol×K	856.06	Joback Method
cpg	829.68	J/mol×K	887.06	Joback Method
cpg	838.77	J/mol×K	918.06	Joback Method
cpg	847.17	J/mol×K	949.06	Joback Method
cpg	854.93	J/mol×K	980.06	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391722&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
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