Glutaric acid, (2-chlorocyclohexyl)methyl 2,2,3,3,4,4,5,5-octafluoropentyl ester

Inchi: InChI=1S/C17H21ClF8O4/c18-11-5-2-1-4-10(11)8-29-12(27)6-3-7-13(28)30-9-15(21,22)1

InchiKey: SNMKZQDBSIBTRX-UHFFFAOYSA-N

Formula: C17H21ClF8O4

SMILES: O=C(CCCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F)OCC1CCCCC1Cl

Mol. weight [g/mol]: 476.79

Physical Properties

Property code	Value	Unit	Source
gf	-1923.17	kJ/mol	Joback Method
hf	-2465.98	kJ/mol	Joback Method
hfus	41.34	kJ/mol	Joback Method
hvap	65.44	kJ/mol	Joback Method
log10ws	-5.84		Crippen Method
logp	5.212		Crippen Method
mcvol	280.810	ml/mol	McGowan Method
pc	1174.44	kPa	Joback Method
rinpol	2107.00		NIST Webbook
rinpol	2107.00		NIST Webbook
tb	777.28	K	Joback Method
tc	958.79	K	Joback Method
tf	455.71	K	Joback Method
vc	1.121	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	886.75	J/mol×K	777.28	Joback Method
cpg	901.52	J/mol×K	807.53	Joback Method
cpg	915.23	J/mol×K	837.78	Joback Method
cpg	927.94	J/mol×K	868.03	Joback Method
cpg	939.70	J/mol×K	898.28	Joback Method
cpg	950.55	J/mol×K	928.54	Joback Method
cpg	960.56	J/mol×K	958.79	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=U405440&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