Glutaric acid, 2,2,3,3,4,4,5,5-octafluoropentyl 2-chloro-6-fluorophenyl ester

Inchi: InChI=1S/C16H12ClF9O4/c17-8-3-1-4-9(18)12(8)30-11(28)6-2-5-10(27)29-7-14(21,22)16

InchiKey: KXCVZMWZNPNQKP-UHFFFAOYSA-N

Formula: C16H12ClF9O4

SMILES: O=C(CCCC(=O)Oc1c(F)cccc1Cl)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 474.70

Physical Properties

Property code	Value	Unit	Source
gf	-2049.99	kJ/mol	Joback Method
hf	-2461.84	kJ/mol	Joback Method
hfus	42.18	kJ/mol	Joback Method
hvap	65.88	kJ/mol	Joback Method
log10ws	-6.27		Crippen Method
logp	5.269		Crippen Method
mcvol	255.590	ml/mol	McGowan Method
pc	1333.93	kPa	Joback Method
rinpol	1947.00		NIST Webbook
rinpol	1947.00		NIST Webbook
tb	775.43	K	Joback Method
tc	957.40	K	Joback Method
tf	493.35	K	Joback Method
vc	1.044	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	749.58	J/mol×K	775.43	Joback Method
cpg	760.32	J/mol×K	805.76	Joback Method
cpg	770.26	J/mol×K	836.09	Joback Method
cpg	779.43	J/mol×K	866.41	Joback Method
cpg	787.90	J/mol×K	896.74	Joback Method
cpg	795.70	J/mol×K	927.07	Joback Method
cpg	802.89	J/mol×K	957.40	Joback Method

Sources

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=U391577&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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