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

Inchi: InChI=1S/C16H13ClF8O4/c17-9-3-1-4-10(7-9)29-12(27)6-2-5-11(26)28-8-14(20,21)16(24

InchiKey: IRLSFNOKJOQTON-UHFFFAOYSA-N

Formula: C16H13ClF8O4

SMILES: O=C(CCCC(=O)Oc1cccc(Cl)c1)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 456.71

Physical Properties

Property code	Value	Unit	Source
gf	-1845.55	kJ/mol	Joback Method
hf	-2254.26	kJ/mol	Joback Method
hfus	39.49	kJ/mol	Joback Method
hvap	66.03	kJ/mol	Joback Method
log10ws	-5.94		Crippen Method
logp	5.130		Crippen Method
mcvol	253.820	ml/mol	McGowan Method
pc	1394.37	kPa	Joback Method
rinpol	2007.00		NIST Webbook
rinpol	2007.00		NIST Webbook
tb	771.18	K	Joback Method
tc	955.87	K	Joback Method
tf	480.24	K	Joback Method
vc	1.026	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	743.13	J/mol×K	771.18	Joback Method
cpg	754.27	J/mol×K	801.96	Joback Method
cpg	764.56	J/mol×K	832.74	Joback Method
cpg	774.06	J/mol×K	863.52	Joback Method
cpg	782.81	J/mol×K	894.30	Joback Method
cpg	790.89	J/mol×K	925.09	Joback Method
cpg	798.34	J/mol×K	955.87	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390455&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

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