Glutaric acid, 3-chlorophenyl 2,2,3,4,4,4-hexafluorobutyl ester

Inchi: InChI=1S/C15H13ClF6O4/c16-9-3-1-4-10(7-9)26-12(24)6-2-5-11(23)25-8-14(18,19)13(17

InchiKey: FAWGFUNBZDUGTL-UHFFFAOYSA-N

Formula: C15H13ClF6O4

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

Mol. weight [g/mol]: 406.70

Physical Properties

Property code	Value	Unit	Source
gf	-1467.19	kJ/mol	Joback Method
hf	-1832.65	kJ/mol	Joback Method
hfus	38.16	kJ/mol	Joback Method
hvap	66.74	kJ/mol	Joback Method
log10ws	-5.20		Crippen Method
logp	4.495		Crippen Method
mcvol	236.190	ml/mol	McGowan Method
pc	1586.01	kPa	Joback Method
rinpol	1900.00		NIST Webbook
rinpol	1900.00		NIST Webbook
tb	752.99	K	Joback Method
tc	941.04	K	Joback Method
tf	465.37	K	Joback Method
vc	0.945	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	671.59	J/mol×K	752.99	Joback Method
cpg	683.00	J/mol×K	784.33	Joback Method
cpg	693.57	J/mol×K	815.67	Joback Method
cpg	703.34	J/mol×K	847.02	Joback Method
cpg	712.34	J/mol×K	878.36	Joback Method
cpg	720.62	J/mol×K	909.70	Joback Method
cpg	728.22	J/mol×K	941.04	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393693&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