Glutaric acid, 3-chlorophenyl pentafluorobenzyl ester

Inchi: InChI=1S/C18H12ClF5O4/c19-9-3-1-4-10(7-9)28-13(26)6-2-5-12(25)27-8-11-14(20)16(22
InchiKey: FULGMPMOTRLWGS-UHFFFAOYSA-N
Formula: C18H12ClF5O4
SMILES: O=C(CCCC(=O)Oc1cccc(Cl)c1)OCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 422.73

Physical Properties

Property code	Value	Unit	Source
gf	-1186.10	kJ/mol	Joback Method
hf	-1496.50	kJ/mol	Joback Method
hfus	53.29	kJ/mol	Joback Method
hvap	82.80	kJ/mol	Joback Method
log10ws	-6.78		Crippen Method
logp	4.855		Crippen Method
mcvol	252.930	ml/mol	McGowan Method
pc	1545.13	kPa	Joback Method
rinpol	2385.00		NIST Webbook
rinpol	2385.00		NIST Webbook
tb	880.84	K	Joback Method
tc	1087.81	K	Joback Method
tf	597.77	K	Joback Method
vc	1.014	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	720.72	J/mol×K	880.84	Joback Method
cpg	730.81	J/mol×K	915.34	Joback Method
cpg	739.90	J/mol×K	949.83	Joback Method
cpg	747.99	J/mol×K	984.33	Joback Method
cpg	755.08	J/mol×K	1018.82	Joback Method
cpg	761.19	J/mol×K	1053.32	Joback Method
cpg	766.31	J/mol×K	1087.81	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391938&Units=SI

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