Glutaric acid, 2,2,3,3-tetrafluoropropyl 3-nitrobenzyl ester

Inchi: InChI=1S/C15H15F4NO6/c16-14(17)15(18,19)9-26-13(22)6-2-5-12(21)25-8-10-3-1-4-11(

InchiKey: VNMCKXNEUTYEFV-UHFFFAOYSA-N

Formula: C15H15F4NO6

SMILES: O=C(CCCC(=O)OCC(F)(F)C(F)F)OCc1cccc([N+](=O)[O-])c1

Mol. weight [g/mol]: 381.28

Physical Properties

Property code	Value	Unit	Source
gf	-1032.93	kJ/mol	Joback Method
hf	-1426.70	kJ/mol	Joback Method
hfus	46.58	kJ/mol	Joback Method
hvap	81.87	kJ/mol	Joback Method
log10ws	-4.70		Crippen Method
logp	3.252		Crippen Method
mcvol	237.830	ml/mol	McGowan Method
pc	1749.21	kPa	Joback Method
rinpol	2305.00		NIST Webbook
rinpol	2305.00		NIST Webbook
tb	872.09	K	Joback Method
tc	1082.52	K	Joback Method
tf	575.46	K	Joback Method
vc	0.953	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	729.46	J/mol×K	872.09	Joback Method
cpg	739.97	J/mol×K	907.16	Joback Method
cpg	749.51	J/mol×K	942.23	Joback Method
cpg	758.10	J/mol×K	977.30	Joback Method
cpg	765.80	J/mol×K	1012.38	Joback Method
cpg	772.64	J/mol×K	1047.45	Joback Method
cpg	778.66	J/mol×K	1082.52	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=U393353&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