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

Inchi: InChI=1S/C14H13F4NO6/c15-13(16)14(17,18)8-24-11(20)6-3-7-12(21)25-10-5-2-1-4-9(1

InchiKey: MCOURDCQJUNWRI-UHFFFAOYSA-N

Formula: C14H13F4NO6

SMILES: O=C(CCCC(=O)Oc1ccccc1[N+](=O)[O-])OCC(F)(F)C(F)F

Mol. weight [g/mol]: 367.25

Physical Properties

Property code	Value	Unit	Source
gf	-1041.35	kJ/mol	Joback Method
hf	-1406.06	kJ/mol	Joback Method
hfus	43.99	kJ/mol	Joback Method
hvap	79.65	kJ/mol	Joback Method
log10ws	-4.44		Crippen Method
logp	3.114		Crippen Method
mcvol	223.740	ml/mol	McGowan Method
pc	1898.60	kPa	Joback Method
rinpol	2108.00		NIST Webbook
rinpol	2108.00		NIST Webbook
tb	849.21	K	Joback Method
tc	1059.85	K	Joback Method
tf	564.19	K	Joback Method
vc	0.896	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	674.23	J/mol×K	849.21	Joback Method
cpg	684.45	J/mol×K	884.32	Joback Method
cpg	693.72	J/mol×K	919.42	Joback Method
cpg	702.07	J/mol×K	954.53	Joback Method
cpg	709.55	J/mol×K	989.64	Joback Method
cpg	716.19	J/mol×K	1024.74	Joback Method
cpg	722.03	J/mol×K	1059.85	Joback Method

Sources

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=U393311&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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