Glutaric acid, 1,1,1-trifluoroprop-2-yl 4-nitrophenyl ester

Inchi: InChI=1S/C14H14F3NO6/c1-9(14(15,16)17)23-12(19)3-2-4-13(20)24-11-7-5-10(6-8-11)1

InchiKey: POWGWGBDPFUTKG-UHFFFAOYSA-N

Formula: C14H14F3NO6

SMILES: CC(OC(=O)CCCC(=O)Oc1ccc([N+](=O)[O-])cc1)C(F)(F)F

Mol. weight [g/mol]: 349.26

Physical Properties

Property code	Value	Unit	Source
gf	-846.54	kJ/mol	Joback Method
hf	-1209.95	kJ/mol	Joback Method
hfus	40.91	kJ/mol	Joback Method
hvap	80.46	kJ/mol	Joback Method
log10ws	-4.58		Crippen Method
logp	3.164		Crippen Method
mcvol	221.970	ml/mol	McGowan Method
pc	1975.31	kPa	Joback Method
rinpol	2090.00		NIST Webbook
rinpol	2090.00		NIST Webbook
tb	849.94	K	Joback Method
tc	1066.37	K	Joback Method
tf	563.60	K	Joback Method
vc	0.878	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	666.76	J/mol×K	849.94	Joback Method
cpg	677.37	J/mol×K	886.01	Joback Method
cpg	686.98	J/mol×K	922.08	Joback Method
cpg	695.63	J/mol×K	958.16	Joback Method
cpg	703.37	J/mol×K	994.23	Joback Method
cpg	710.22	J/mol×K	1030.30	Joback Method
cpg	716.23	J/mol×K	1066.37	Joback Method

Sources

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=U391966&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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