Glutaric acid, 1,1,1-trifluoroprop-2-yl 3-nitrobenzyl ester

Inchi: InChI=1S/C15H16F3NO6/c1-10(15(16,17)18)25-14(21)7-3-6-13(20)24-9-11-4-2-5-12(8-1

InchiKey: XLNKOSULOGOSHJ-UHFFFAOYSA-N

Formula: C15H16F3NO6

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

Mol. weight [g/mol]: 363.29

Physical Properties

Property code	Value	Unit	Source
gf	-838.12	kJ/mol	Joback Method
hf	-1230.59	kJ/mol	Joback Method
hfus	43.50	kJ/mol	Joback Method
hvap	82.69	kJ/mol	Joback Method
log10ws	-4.85		Crippen Method
logp	3.302		Crippen Method
mcvol	236.060	ml/mol	McGowan Method
pc	1816.95	kPa	Joback Method
rinpol	2209.00		NIST Webbook
rinpol	2209.00		NIST Webbook
tb	872.82	K	Joback Method
tc	1088.31	K	Joback Method
tf	574.87	K	Joback Method
vc	0.934	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	722.09	J/mol×K	872.82	Joback Method
cpg	732.97	J/mol×K	908.74	Joback Method
cpg	742.82	J/mol×K	944.65	Joback Method
cpg	751.70	J/mol×K	980.57	Joback Method
cpg	759.64	J/mol×K	1016.48	Joback Method
cpg	766.69	J/mol×K	1052.40	Joback Method
cpg	772.88	J/mol×K	1088.31	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393352&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