Glutaric acid, 2,2,3,3,4,4,5,5-octafluoropentyl 3-nitrobenzyl ester

Inchi: InChI=1S/C17H15F8NO6/c18-14(19)16(22,23)17(24,25)15(20,21)9-32-13(28)6-2-5-12(2
InchiKey: CJWIVYYHRFQQCL-UHFFFAOYSA-N
Formula: C17H15F8NO6
SMILES: O=C(CCCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F)OCc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]: 481.29

Physical Properties

Property code	Value	Unit	Source
gf	-1789.65	kJ/mol	Joback Method
hf	-2269.92	kJ/mol	Joback Method
hfus	49.25	kJ/mol	Joback Method
hvap	80.46	kJ/mol	Joback Method
log10ws	-6.17		Crippen Method
logp	4.522		Crippen Method
mcvol	273.090	ml/mol	McGowan Method
pc	1346.69	kPa	Joback Method
rinpol	2376.00		NIST Webbook
rinpol	2376.00		NIST Webbook
tb	908.47	K	Joback Method
tc	1115.37	K	Joback Method
tf	605.20	K	Joback Method
vc	1.115	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	872.95	J/mol×K	908.47	Joback Method
cpg	882.93	J/mol×K	942.95	Joback Method
cpg	892.04	J/mol×K	977.44	Joback Method
cpg	900.39	J/mol×K	1011.92	Joback Method
cpg	908.04	J/mol×K	1046.40	Joback Method
cpg	915.09	J/mol×K	1080.89	Joback Method
cpg	921.61	J/mol×K	1115.37	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393354&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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