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

Inchi: InChI=1S/C16H13F8NO6/c17-13(18)15(21,22)16(23,24)14(19,20)8-30-11(26)6-3-7-12(2
InchiKey: OGJBFRZHXVSFIY-UHFFFAOYSA-N
Formula: C16H13F8NO6
SMILES: O=C(CCCC(=O)Oc1ccccc1[N+](=O)[O-])OCC(F)(F)C(F)(F)C(F)(F)C(F)F
Mol. weight [g/mol]: 467.26

Physical Properties

Property code	Value	Unit	Source
gf	-1798.07	kJ/mol	Joback Method
hf	-2249.28	kJ/mol	Joback Method
hfus	46.66	kJ/mol	Joback Method
hvap	78.24	kJ/mol	Joback Method
log10ws	-5.90		Crippen Method
logp	4.385		Crippen Method
mcvol	259.000	ml/mol	McGowan Method
pc	1446.83	kPa	Joback Method
rinpol	2184.00		NIST Webbook
rinpol	2184.00		NIST Webbook
tb	885.59	K	Joback Method
tc	1090.18	K	Joback Method
tf	593.93	K	Joback Method
vc	1.058	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	816.99	J/mol×K	885.59	Joback Method
cpg	826.59	J/mol×K	919.69	Joback Method
cpg	835.34	J/mol×K	953.79	Joback Method
cpg	843.33	J/mol×K	987.89	Joback Method
cpg	850.62	J/mol×K	1021.99	Joback Method
cpg	857.31	J/mol×K	1056.09	Joback Method
cpg	863.47	J/mol×K	1090.18	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=U393312&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