Succinic acid, 5-fluoro-2-nitrophenyl 2,2,3,3,4,4,4-heptafluorobutyl ester

Inchi: InChI=1S/C14H9F8NO6/c15-7-1-2-8(23(26)27)9(5-7)29-11(25)4-3-10(24)28-6-12(16,17)

InchiKey: OVVQIRADYXWKMH-UHFFFAOYSA-N

Formula: C14H9F8NO6

SMILES: O=C(CCC(=O)Oc1cc(F)ccc1[N+](=O)[O-])OCC(F)(F)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 439.21

Physical Properties

Property code	Value	Unit	Source
gf	-1822.10	kJ/mol	Joback Method
hf	-2214.19	kJ/mol	Joback Method
hfus	44.61	kJ/mol	Joback Method
hvap	74.84	kJ/mol	Joback Method
log10ws	-5.43		Crippen Method
logp	3.796		Crippen Method
mcvol	230.820	ml/mol	McGowan Method
pc	1652.46	kPa	Joback Method
rinpol	1877.00		NIST Webbook
tb	845.25	K	Joback Method
tc	1046.66	K	Joback Method
tf	598.91	K	Joback Method
vc	0.953	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	705.16	J/mol×K	845.25	Joback Method
cpg	713.89	J/mol×K	878.82	Joback Method
cpg	721.81	J/mol×K	912.39	Joback Method
cpg	729.01	J/mol×K	945.95	Joback Method
cpg	735.55	J/mol×K	979.52	Joback Method
cpg	741.48	J/mol×K	1013.09	Joback Method
cpg	746.87	J/mol×K	1046.66	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=U357979&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