Succinic acid, 2-fluoro-5-nitrobenzyl hexyl ester

Inchi: InChI=1S/C17H22FNO6/c1-2-3-4-5-10-24-16(20)8-9-17(21)25-12-13-11-14(19(22)23)6-7

InchiKey: OCWAEHORVVIPCD-UHFFFAOYSA-N

Formula: C17H22FNO6

SMILES: CCCCCCOC(=O)CCC(=O)OCc1cc([N+](=O)[O-])ccc1F

Mol. weight [g/mol]: 355.36

Physical Properties

Property code	Value	Unit	Source
gf	-441.69	kJ/mol	Joback Method
hf	-877.09	kJ/mol	Joback Method
hfus	53.06	kJ/mol	Joback Method
hvap	91.12	kJ/mol	Joback Method
log10ws	-5.24		Crippen Method
logp	3.681		Crippen Method
mcvol	260.700	ml/mol	McGowan Method
pc	1612.88	kPa	Joback Method
rinpol	2517.00		NIST Webbook
rinpol	2517.00		NIST Webbook
tb	928.69	K	Joback Method
tc	1147.20	K	Joback Method
tf	621.33	K	Joback Method
vc	1.028	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	818.15	J/mol×K	928.69	Joback Method
cpg	829.93	J/mol×K	965.11	Joback Method
cpg	840.53	J/mol×K	1001.53	Joback Method
cpg	849.96	J/mol×K	1037.94	Joback Method
cpg	858.24	J/mol×K	1074.36	Joback Method
cpg	865.39	J/mol×K	1110.78	Joback Method
cpg	871.44	J/mol×K	1147.20	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=U380928&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