

Succinic acid, 2-fluorophenyl neopentyl ester

Inchi: InChI=1S/C15H19FO4/c1-15(2,3)10-19-13(17)8-9-14(18)20-12-7-5-4-6-11(12)16/h4-7H,8
InchiKey: GPANKRLKKJTRFW-UHFFFAOYSA-N
Formula: C15H19FO4
SMILES: CC(C)(C)COC(=O)CCC(=O)Oc1ccccc1F
Mol. weight [g/mol]: 282.31

Physical Properties

Property code	Value	Unit	Source
gf	-481.61	kJ/mol	Joback Method
hf	-822.33	kJ/mol	Joback Method
hfus	29.50	kJ/mol	Joback Method
hvap	68.12	kJ/mol	Joback Method
log10ws	-3.67		Crippen Method
logp	3.101		Crippen Method
mvol	215.100	ml/mol	McGowan Method
pc	1930.44	kPa	Joback Method
rinpol	1828.00		NIST Webbook
rinpol	1828.00		NIST Webbook
tb	722.88	K	Joback Method
tc	928.08	K	Joback Method
tf	445.08	K	Joback Method
vc	0.823	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	603.88	J/mol×K	722.88	Joback Method
cpg	618.42	J/mol×K	757.08	Joback Method
cpg	631.98	J/mol×K	791.28	Joback Method
cpg	644.59	J/mol×K	825.48	Joback Method
cpg	656.28	J/mol×K	859.68	Joback Method
cpg	667.08	J/mol×K	893.88	Joback Method
cpg	677.01	J/mol×K	928.08	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U389582&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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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