

Succinic acid, 2-fluorophenethyl isobutyl ester

Inchi: InChI=1S/C16H21FO4/c1-12(2)11-21-16(19)8-7-15(18)20-10-9-13-5-3-4-6-14(13)17/h3-6
InchiKey: IBIGQPLPRIMGIM-UHFFFAOYSA-N
Formula: C16H21FO4
SMILES: CC(C)COC(=O)CCC(=O)OCCc1ccccc1F
Mol. weight [g/mol]: 296.33

Physical Properties

Property code	Value	Unit	Source
gf	-478.47	kJ/mol	Joback Method
hf	-839.50	kJ/mol	Joback Method
hfus	35.98	kJ/mol	Joback Method
hvap	71.26	kJ/mol	Joback Method
log10ws	-3.44		Crippen Method
logp	2.891		Crippen Method
mcvol	229.190	ml/mol	McGowan Method
pc	1760.97	kPa	Joback Method
rinpola	1990.00		NIST Webbook
rinpola	1990.00		NIST Webbook
tb	748.55	K	Joback Method
tc	946.59	K	Joback Method
tf	438.93	K	Joback Method
vc	0.883	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	656.73	J/molxK	748.55	Joback Method
cpg	671.50	J/molxK	781.56	Joback Method
cpg	685.32	J/molxK	814.56	Joback Method
cpg	698.20	J/molxK	847.57	Joback Method
cpg	710.16	J/molxK	880.57	Joback Method
cpg	721.20	J/molxK	913.58	Joback Method
cpg	731.34	J/molxK	946.59	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381400&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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