

Succinic acid, 2-fluorophenyl 2,3,4-trifluorophenyl ester

Inchi: InChI=1S/C16H10F4O4/c17-9-3-1-2-4-11(9)23-13(21)7-8-14(22)24-12-6-5-10(18)15(19)
InchiKey: ZDLABVVFLIDSMY-UHFFFAOYSA-N
Formula: C16H10F4O4
SMILES: O=C(CCC(=O)Oc1ccc(F)c(F)c1F)Oc1ccccc1F
Mol. weight [g/mol]: 342.24

Physical Properties

Property code	Value	Unit	Source
gf	-976.94	kJ/mol	Joback Method
hf	-1220.43	kJ/mol	Joback Method
hfus	41.62	kJ/mol	Joback Method
hvap	73.45	kJ/mol	Joback Method
log10ws	-5.07		Crippen Method
logp	3.534		Crippen Method
mcvol	210.740	ml/mol	McGowan Method
pc	1992.98	kPa	Joback Method
rinpol	2105.00		NIST Webbook
rinpol	2105.00		NIST Webbook
tb	788.42	K	Joback Method
tc	994.77	K	Joback Method
tf	519.68	K	Joback Method
vc	0.836	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	585.08	J/mol×K	788.42	Joback Method
cpg	596.15	J/mol×K	822.81	Joback Method
cpg	606.31	J/mol×K	857.20	Joback Method
cpg	615.56	J/mol×K	891.60	Joback Method
cpg	623.92	J/mol×K	925.99	Joback Method
cpg	631.39	J/mol×K	960.38	Joback Method
cpg	637.97	J/mol×K	994.77	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=U390762&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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