

Glutaric acid, 2-norbornyl 2-fluorophenyl ester

Inchi: InChI=1S/C18H21FO4/c19-14-4-1-2-5-15(14)22-17(20)6-3-7-18(21)23-16-11-12-8-9-13(20)/1
InchiKey: UUIIPDWNAPDCKX-UHFFFAOYSA-N
Formula: C18H21FO4
SMILES: O=C(CCCC(=O)OC1CC2CCC1C2)Oc1ccccc1F
Mol. weight [g/mol]: 320.36

Physical Properties

Property code	Value	Unit	Source
gf	-357.50	kJ/mol	Joback Method
hf	-756.40	kJ/mol	Joback Method
hfus	39.92	kJ/mol	Joback Method
hvap	75.78	kJ/mol	Joback Method
log10ws	-4.58		Crippen Method
logp	3.633		Crippen Method
mcvol	235.650	ml/mol	McGowan Method
pc	1840.41	kPa	Joback Method
rinpola	2338.00		NIST Webbook
rinpola	2338.00		NIST Webbook
tb	807.83	K	Joback Method
tc	1024.02	K	Joback Method
tf	504.59	K	Joback Method
vc	0.906	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	743.11	J/molxK	807.83	Joback Method
cpg	759.25	J/molxK	843.86	Joback Method
cpg	774.22	J/molxK	879.89	Joback Method
cpg	788.08	J/molxK	915.92	Joback Method
cpg	800.88	J/molxK	951.95	Joback Method
cpg	812.69	J/molxK	987.99	Joback Method
cpg	823.58	J/molxK	1024.02	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U405492&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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