

Glutaric acid, butyl 3,5-difluorophenyl ester

Inchi:	InChI=1S/C15H18F2O4/c1-2-3-7-20-14(18)5-4-6-15(19)21-13-9-11(16)8-12(17)10-13/h8
InchiKey:	HSKLIYWHMNVGTA-UHFFFAOYSA-N
Formula:	C15H18F2O4
SMILES:	CCCCOC(=O)CCCC(=O)Oc1cc(F)cc(F)c1
Mol. weight [g/mol]:	300.30

Physical Properties

Property code	Value	Unit	Source
gf	-688.89	kJ/mol	Joback Method
hf	-1021.16	kJ/mol	Joback Method
hfus	39.60	kJ/mol	Joback Method
hvap	69.26	kJ/mol	Joback Method
log10ws	-4.24		Crippen Method
logp	3.384		Crippen Method
mcvol	216.870	ml/mol	McGowan Method
pc	1803.09	kPa	Joback Method
rinpol	1913.00		NIST Webbook
rinpol	1913.00		NIST Webbook
tb	730.36	K	Joback Method
tc	921.52	K	Joback Method
tf	455.77	K	Joback Method
vc	0.852	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	608.38	J/molxK	730.36	Joback Method
cpg	621.95	J/molxK	762.22	Joback Method
cpg	634.70	J/molxK	794.08	Joback Method
cpg	646.64	J/molxK	825.94	Joback Method
cpg	657.77	J/molxK	857.80	Joback Method
cpg	668.10	J/molxK	889.66	Joback Method
cpg	677.64	J/molxK	921.52	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=U358628&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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