

Glutaric acid, ethyl 4-fluoro-2-methoxyphenyl ester

Inchi:	InChI=1S/C14H17FO5/c1-3-19-13(16)5-4-6-14(17)20-11-8-7-10(15)9-12(11)18-2/h7-9H,1
InchiKey:	GESBKZQPLMNBMG-UHFFFAOYSA-N
Formula:	C14H17FO5
SMILES:	CCOC(=O)CCCC(=O)Oc1ccc(F)cc1OC
Mol. weight [g/mol]:	284.28

Physical Properties

Property code	Value	Unit	Source
gf	-607.50	kJ/mol	Joback Method
hf	-936.63	kJ/mol	Joback Method
hfus	35.12	kJ/mol	Joback Method
hvap	70.26	kJ/mol	Joback Method
log10ws	-3.19		Crippen Method
logp	2.473		Crippen Method
mcvol	206.880	ml/mol	McGowan Method
pc	2009.10	kPa	Joback Method
rinpola	1905.00		NIST Webbook
rinpola	1905.00		NIST Webbook
tb	730.63	K	Joback Method
tc	928.80	K	Joback Method
tf	466.14	K	Joback Method
vc	0.795	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	573.48	J/mol×K	730.63	Joback Method
cpg	586.88	J/mol×K	763.66	Joback Method
cpg	599.44	J/mol×K	796.69	Joback Method
cpg	611.14	J/mol×K	829.72	Joback Method
cpg	621.99	J/mol×K	862.75	Joback Method
cpg	631.96	J/mol×K	895.78	Joback Method
cpg	641.05	J/mol×K	928.80	Joback Method

Sources

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=U393573&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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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