

Glutaric acid, di(4-fluoro-2-methoxyphenyl) ester

Inchi:	InChI=1S/C19H18F2O6/c1-24-16-10-12(20)6-8-14(16)26-18(22)4-3-5-19(23)27-15-9-7-1
InchiKey:	ARQVKJJYNWLLDY-UHFFFAOYSA-N
Formula:	C19H18F2O6
SMILES:	COc1cc(F)ccc1OC(=O)CCCC(=O)Oc1ccc(F)cc1OC
Mol. weight [g/mol]:	380.34

Physical Properties

Property code	Value	Unit	Source
gf	-772.06	kJ/mol	Joback Method
hf	-1154.57	kJ/mol	Joback Method
hfus	45.60	kJ/mol	Joback Method
hvap	86.59	kJ/mol	Joback Method
log10ws	-5.07		Crippen Method
logp	3.663		Crippen Method
mcvol	261.210	ml/mol	McGowan Method
pc	1636.45	kPa	Joback Method
rinpola	2619.00		NIST Webbook
rinpola	2619.00		NIST Webbook
tb	903.36	K	Joback Method
tc	1118.91	K	Joback Method
tf	596.77	K	Joback Method
vc	1.004	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	788.62	J/mol×K	903.36	Joback Method
cpg	800.14	J/mol×K	939.28	Joback Method
cpg	810.30	J/mol×K	975.21	Joback Method
cpg	819.10	J/mol×K	1011.13	Joback Method
cpg	826.51	J/mol×K	1047.06	Joback Method
cpg	832.52	J/mol×K	1082.98	Joback Method
cpg	837.12	J/mol×K	1118.91	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U393572&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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