

Glutaric acid, 2-chloro-6-fluorophenyl 3-ethylphenyl ester

Inchi:	InChI=1S/C19H18ClFO4/c1-2-13-6-3-7-14(12-13)24-17(22)10-5-11-18(23)25-19-15(20)8
InchiKey:	RTEPWBMUAUCHGIO-UHFFFAOYSA-N
Formula:	C19H18ClFO4
SMILES:	CCc1cccc(OC(=O)CCCC(=O)Oc2c(F)cccc2Cl)c1
Mol. weight [g/mol]:	364.80

Physical Properties

Property code	Value	Unit	Source
gf	-369.55	kJ/mol	Joback Method
hf	-698.29	kJ/mol	Joback Method
hfus	44.73	kJ/mol	Joback Method
hvap	86.31	kJ/mol	Joback Method
log10ws	-5.99		Crippen Method
logp	4.723		Crippen Method
mvol	259.940	ml/mol	McGowan Method
pc	1714.61	kPa	Joback Method
rinpol	2608.00		NIST Webbook
rinpol	2608.00		NIST Webbook
tb	891.70	K	Joback Method
tc	1115.74	K	Joback Method
tf	569.12	K	Joback Method
vc	0.999	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	752.15	J/molxK	891.70	Joback Method
cpg	764.19	J/molxK	929.04	Joback Method
cpg	775.02	J/molxK	966.38	Joback Method
cpg	784.67	J/molxK	1003.72	Joback Method
cpg	793.18	J/molxK	1041.06	Joback Method
cpg	800.55	J/molxK	1078.40	Joback Method
cpg	806.82	J/molxK	1115.74	Joback Method

Sources

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=U391508&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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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