

Glutaric acid, 2-chloro-6-fluorophenyl 4-methylpent-2-yl ester

Inchi:	InChI=1S/C17H22ClFO4/c1-11(2)10-12(3)22-15(20)8-5-9-16(21)23-17-13(18)6-4-7-14(1)
InchiKey:	NBJSFJYRCDBVEC-UHFFFAOYSA-N
Formula:	C17H22ClFO4
SMILES:	CC(C)CC(C)OC(=O)CCCC(=O)Oc1c(F)cccc1Cl
Mol. weight [g/mol]:	344.81

Physical Properties

Property code	Value	Unit	Source
gf	-494.05	kJ/mol	Joback Method
hf	-892.63	kJ/mol	Joback Method
hfus	38.85	kJ/mol	Joback Method
hvap	78.14	kJ/mol	Joback Method
log10ws	-5.30		Crippen Method
logp	4.533		Crippen Method
mvol	255.520	ml/mol	McGowan Method
pc	1570.96	kPa	Joback Method
rinpol	2132.00		NIST Webbook
rinpol	2132.00		NIST Webbook
tb	813.40	K	Joback Method
tc	1017.91	K	Joback Method
tf	477.64	K	Joback Method
vc	0.983	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	739.00	J/mol×K	813.40	Joback Method
cpg	753.03	J/mol×K	847.48	Joback Method
cpg	766.01	J/mol×K	881.57	Joback Method
cpg	777.97	J/mol×K	915.65	Joback Method
cpg	788.91	J/mol×K	949.74	Joback Method
cpg	798.85	J/mol×K	983.82	Joback Method
cpg	807.80	J/mol×K	1017.91	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=U392494&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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