

Glutaric acid, 1,1,1-trifluoroprop-2-yl 2-chloro-5-methylphenyl ester

Inchi:	InChI=1S/C15H16ClF3O4/c1-9-6-7-11(16)12(8-9)23-14(21)5-3-4-13(20)22-10(2)15(17,18)
InchiKey:	BYTVYKBF3CGBXJU-UHFFFAOYSA-N
Formula:	C15H16ClF3O4
SMILES:	<chem>Cc1ccc(Cl)c(OC(=O)CCCC(=O)OC(C)C(F)(F)F)c1</chem>
Mol. weight [g/mol]:	352.73

Physical Properties

Property code	Value	Unit	Source
gf	-895.23	kJ/mol	Joback Method
hf	-1247.04	kJ/mol	Joback Method
hfus	35.94	kJ/mol	Joback Method
hvap	71.15	kJ/mol	Joback Method
log10ws	-5.09		Crippen Method
logp	4.218		Crippen Method
mvol	230.880	ml/mol	McGowan Method
pc	1721.73	kPa	Joback Method
rinpol	1924.00		NIST Webbook
rinpol	1924.00		NIST Webbook
tb	763.39	K	Joback Method
tc	962.40	K	Joback Method
tf	473.70	K	Joback Method
vc	0.901	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	644.84	J/molxK	763.39	Joback Method
cpg	657.30	J/molxK	796.56	Joback Method
cpg	668.87	J/molxK	829.73	Joback Method
cpg	679.57	J/molxK	862.90	Joback Method
cpg	689.42	J/molxK	896.06	Joback Method
cpg	698.46	J/molxK	929.23	Joback Method
cpg	706.70	J/molxK	962.40	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=U393413&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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