Glutaric acid, 3-methylbut-2-en-1-yl 2-chloro-6-fluorophenyl ester

Inchi: InChI=1S/C16H18ClFO4/c1-11(2)9-10-21-14(19)7-4-8-15(20)22-16-12(17)5-3-6-13(16)18

InchiKey: IORYZGQIHYMTRN-UHFFFAOYSA-N

Formula: C16H18ClFO4

SMILES: CC(C)=CCOC(=O)CCCC(=O)Oc1c(F)cccc1Cl

Mol. weight [g/mol]: 328.76

Physical Properties

Property code	Value	Unit	Source
gf	-425.92	kJ/mol	Joback Method
hf	-754.00	kJ/mol	Joback Method
hfus	42.20	kJ/mol	Joback Method
hvap	76.73	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	4.064		Crippen Method
mcvol	237.130	ml/mol	McGowan Method
pc	1756.54	kPa	Joback Method
rinpol	2190.00		NIST Webbook
rinpol	2190.00		NIST Webbook
tb	795.44	K	Joback Method
tc	1003.51	K	Joback Method
tf	477.33	K	Joback Method
vc	0.919	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	655.71	J/mol×K	795.44	Joback Method
cpg	668.73	J/mol×K	830.12	Joback Method
cpg	680.83	J/mol×K	864.80	Joback Method
cpg	692.04	J/mol×K	899.48	Joback Method
cpg	702.38	J/mol×K	934.15	Joback Method
cpg	711.88	J/mol×K	968.83	Joback Method
cpg	720.54	J/mol×K	1003.51	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=U391581&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
hvap:	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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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