Glutaric acid, 1,1,1-trifluoroprop-2-yl 2-formylphenyl ester

Inchi: InChI=1S/C15H15F3O5/c1-10(15(16,17)18)22-13(20)7-4-8-14(21)23-12-6-3-2-5-11(12)9

InchiKey: ZOJSRBZDCBRVTP-UHFFFAOYSA-N

Formula: C15H15F3O5

SMILES: CC(OC(=O)CCCC(=O)Oc1ccccc1C=O)C(F)(F)F

Mol. weight [g/mol]: 332.27

Physical Properties

Property code	Value	Unit	Source
gf	-973.19	kJ/mol	Joback Method
hf	-1305.41	kJ/mol	Joback Method
hfus	34.42	kJ/mol	Joback Method
hvap	72.82	kJ/mol	Joback Method
log10ws	-4.18		Crippen Method
logp	3.069		Crippen Method
mcvol	220.210	ml/mol	McGowan Method
pc	1916.94	kPa	Joback Method
rinpol	1941.00		NIST Webbook
tb	769.64	K	Joback Method
tc	967.65	K	Joback Method
tf	473.26	K	Joback Method
vc	0.870	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	635.20	J/mol×K	769.64	Joback Method
cpg	647.11	J/mol×K	802.64	Joback Method
cpg	658.13	J/mol×K	835.64	Joback Method
cpg	668.29	J/mol×K	868.64	Joback Method
cpg	677.60	J/mol×K	901.64	Joback Method
cpg	686.11	J/mol×K	934.65	Joback Method
cpg	693.83	J/mol×K	967.65	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=U390490&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