Glutaric acid, 1,1,1-trifluoroprop-2-yl 3-methyl-5-methoxypentyl ester

Inchi: InChI=1S/C15H25F3O5/c1-11(7-9-21-3)8-10-22-13(19)5-4-6-14(20)23-12(2)15(16,17)18

InchiKey: AENBGEZITJXMQF-UHFFFAOYSA-N

Formula: C15H25F3O5

SMILES: COCCC(C)CCOC(=O)CCCC(=O)OC(C)C(F)(F)F

Mol. weight [g/mol]: 342.35

Physical Properties

Property code	Value	Unit	Source
gf	-1083.89	kJ/mol	Joback Method
hf	-1582.39	kJ/mol	Joback Method
hfus	36.15	kJ/mol	Joback Method
hvap	65.18	kJ/mol	Joback Method
log10ws	-3.45		Crippen Method
logp	3.257		Crippen Method
mcvol	248.270	ml/mol	McGowan Method
pc	1389.18	kPa	Joback Method
rinpol	1703.00		NIST Webbook
tb	711.30	K	Joback Method
tc	883.61	K	Joback Method
tf	399.55	K	Joback Method
vc	0.973	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	733.25	J/mol×K	711.30	Joback Method
cpg	748.43	J/mol×K	740.02	Joback Method
cpg	762.81	J/mol×K	768.74	Joback Method
cpg	776.39	J/mol×K	797.46	Joback Method
cpg	789.19	J/mol×K	826.18	Joback Method
cpg	801.21	J/mol×K	854.89	Joback Method
cpg	812.47	J/mol×K	883.61	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U393514&Units=SI

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