Glutaric acid, ethyl 1-phenyl-2,2,2-trifluoroethyl ester

Inchi: InChI=1S/C15H17F3O4/c1-2-21-12(19)9-6-10-13(20)22-14(15(16,17)18)11-7-4-3-5-8-11/

InchiKey: MXUMVQXSIURNCR-UHFFFAOYSA-N

Formula: C15H17F3O4

SMILES: CCOC(=O)CCCC(=O)OC(c1ccccc1)C(F)(F)F

Mol. weight [g/mol]: 318.29

Physical Properties

Property code	Value	Unit	Source
gf	-864.04	kJ/mol	Joback Method
hf	-1208.36	kJ/mol	Joback Method
hfus	32.52	kJ/mol	Joback Method
hvap	65.44	kJ/mol	Joback Method
log10ws	-4.05		Crippen Method
logp	3.567		Crippen Method
mcvol	218.640	ml/mol	McGowan Method
pc	1821.61	kPa	Joback Method
rinpol	1780.00		NIST Webbook
rinpol	1780.00		NIST Webbook
tb	716.00	K	Joback Method
tc	909.33	K	Joback Method
tf	418.74	K	Joback Method
vc	0.853	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	620.97	J/mol×K	716.00	Joback Method
cpg	634.74	J/mol×K	748.22	Joback Method
cpg	647.58	J/mol×K	780.44	Joback Method
cpg	659.52	J/mol×K	812.66	Joback Method
cpg	670.61	J/mol×K	844.89	Joback Method
cpg	680.87	J/mol×K	877.11	Joback Method
cpg	690.33	J/mol×K	909.33	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=U377362&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