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

Inchi: InChI=1S/C15H21F3O4/c1-9(15(16,17)18)21-13(19)3-2-4-14(20)22-12-8-10-5-6-11(12)7

InchiKey: SSDNVZHBAHOKRY-UHFFFAOYSA-N

Formula: C15H21F3O4

SMILES: CC(OC(=O)CCCC(=O)OC1CC2CCC1C2)C(F)(F)F

Mol. weight [g/mol]: 322.32

Physical Properties

Property code	Value	Unit	Source
gf	-874.76	kJ/mol	Joback Method
hf	-1325.79	kJ/mol	Joback Method
hfus	33.72	kJ/mol	Joback Method
hvap	62.85	kJ/mol	Joback Method
log10ws	-4.02		Crippen Method
logp	3.383		Crippen Method
mcvol	220.680	ml/mol	McGowan Method
pc	1704.71	kPa	Joback Method
rinpol	1702.00		NIST Webbook
rinpol	1702.00		NIST Webbook
tb	702.40	K	Joback Method
tc	891.13	K	Joback Method
tf	420.44	K	Joback Method
vc	0.866	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	679.36	J/mol×K	702.40	Joback Method
cpg	695.74	J/mol×K	733.86	Joback Method
cpg	711.13	J/mol×K	765.31	Joback Method
cpg	725.56	J/mol×K	796.77	Joback Method
cpg	739.10	J/mol×K	828.22	Joback Method
cpg	751.79	J/mol×K	859.68	Joback Method
cpg	763.68	J/mol×K	891.13	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405482&Units=SI
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

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