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

Inchi: InChI=1S/C13H21F3O4/c1-9(13(14,15)16)20-11(18)7-5-6-10(17)19-8-12(2,3)4/h9H,5-8H

InchiKey: HSHBFZWBLPTFQT-UHFFFAOYSA-N

Formula: C13H21F3O4

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

Mol. weight [g/mol]: 298.30

Physical Properties

Property code	Value	Unit	Source
gf	-990.45	kJ/mol	Joback Method
hf	-1412.36	kJ/mol	Joback Method
hfus	25.89	kJ/mol	Joback Method
hvap	57.41	kJ/mol	Joback Method
log10ws	-3.52		Crippen Method
logp	3.240		Crippen Method
mcvol	214.220	ml/mol	McGowan Method
pc	1648.43	kPa	Joback Method
rinpol	1370.00		NIST Webbook
rinpol	1370.00		NIST Webbook
tb	640.33	K	Joback Method
tc	815.51	K	Joback Method
tf	372.20	K	Joback Method
vc	0.838	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	598.45	J/mol×K	640.33	Joback Method
cpg	613.10	J/mol×K	669.53	Joback Method
cpg	626.95	J/mol×K	698.72	Joback Method
cpg	640.04	J/mol×K	727.92	Joback Method
cpg	652.38	J/mol×K	757.11	Joback Method
cpg	664.00	J/mol×K	786.31	Joback Method
cpg	674.93	J/mol×K	815.51	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=U391603&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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