Glutaric acid, 1,1,1-trifluoroprop-2-yl 2,4,4-trimethylpentyl ester

Inchi: InChI=1S/C16H27F3O4/c1-11(9-15(3,4)5)10-22-13(20)7-6-8-14(21)23-12(2)16(17,18)19/

InchiKey: VYEYVFHAYPBWEX-UHFFFAOYSA-N

Formula: C16H27F3O4

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

Mol. weight [g/mol]: 340.38

Physical Properties

Property code	Value	Unit	Source
gf	-967.63	kJ/mol	Joback Method
hf	-1479.56	kJ/mol	Joback Method
hfus	30.14	kJ/mol	Joback Method
hvap	63.70	kJ/mol	Joback Method
log10ws	-4.54		Crippen Method
logp	4.266		Crippen Method
mcvol	256.490	ml/mol	McGowan Method
pc	1329.07	kPa	Joback Method
rinpol	1609.00		NIST Webbook
rinpol	1609.00		NIST Webbook
tb	708.53	K	Joback Method
tc	885.31	K	Joback Method
tf	391.01	K	Joback Method
vc	1.000	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	762.13	J/mol×K	708.53	Joback Method
cpg	778.19	J/mol×K	737.99	Joback Method
cpg	793.34	J/mol×K	767.46	Joback Method
cpg	807.62	J/mol×K	796.92	Joback Method
cpg	821.06	J/mol×K	826.38	Joback Method
cpg	833.71	J/mol×K	855.85	Joback Method
cpg	845.58	J/mol×K	885.31	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=U391522&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