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

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

InchiKey: VRNHYFRBKGVSQQ-UHFFFAOYSA-N

Formula: C16H27F3O4

SMILES: CCCCCCC(C)OC(=O)CCCC(=O)OC(C)C(F)(F)F

Mol. weight [g/mol]: 340.38

Physical Properties

Property code	Value	Unit	Source
gf	-970.47	kJ/mol	Joback Method
hf	-1470.81	kJ/mol	Joback Method
hfus	37.55	kJ/mol	Joback Method
hvap	65.00	kJ/mol	Joback Method
log10ws	-5.13		Crippen Method
logp	4.553		Crippen Method
mcvol	256.490	ml/mol	McGowan Method
pc	1310.85	kPa	Joback Method
rinpol	1686.00		NIST Webbook
rinpol	1686.00		NIST Webbook
tb	711.76	K	Joback Method
tc	883.69	K	Joback Method
tf	388.59	K	Joback Method
vc	1.010	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	759.95	J/mol×K	711.76	Joback Method
cpg	775.76	J/mol×K	740.41	Joback Method
cpg	790.74	J/mol×K	769.07	Joback Method
cpg	804.91	J/mol×K	797.72	Joback Method
cpg	818.29	J/mol×K	826.38	Joback Method
cpg	830.90	J/mol×K	855.03	Joback Method
cpg	842.76	J/mol×K	883.69	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=U391443&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