Glutaric acid, 2-(cyclohexyl)ethyl 1,1,1-trifluoroprop-2-yl ester

Inchi: InChI=1S/C16H25F3O4/c1-12(16(17,18)19)23-15(21)9-5-8-14(20)22-11-10-13-6-3-2-4-7

InchiKey: XQZKEAUJMCIKER-UHFFFAOYSA-N

Formula: C16H25F3O4

SMILES: CC(OC(=O)CCCC(=O)OCCC1CCCCC1)C(F)(F)F

Mol. weight [g/mol]: 338.36

Physical Properties

Property code	Value	Unit	Source
gf	-943.58	kJ/mol	Joback Method
hf	-1411.21	kJ/mol	Joback Method
hfus	32.91	kJ/mol	Joback Method
hvap	65.82	kJ/mol	Joback Method
log10ws	-4.67		Crippen Method
logp	4.164		Crippen Method
mcvol	245.630	ml/mol	McGowan Method
pc	1519.94	kPa	Joback Method
rinpol	1779.00		NIST Webbook
rinpol	1779.00		NIST Webbook
tb	731.75	K	Joback Method
tc	919.77	K	Joback Method
tf	410.97	K	Joback Method
vc	0.950	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	754.45	J/mol×K	731.75	Joback Method
cpg	771.58	J/mol×K	763.09	Joback Method
cpg	787.64	J/mol×K	794.42	Joback Method
cpg	802.64	J/mol×K	825.76	Joback Method
cpg	816.62	J/mol×K	857.10	Joback Method
cpg	829.60	J/mol×K	888.43	Joback Method
cpg	841.61	J/mol×K	919.77	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405411&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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