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

Inchi: InChI=1S/C18H25F3O4/c1-11(18(19,20)21)25-16(23)6-4-5-15(22)24-10-12-7-8-13-9-14(

InchiKey: KDPBABZVCVHWMJ-UHFFFAOYSA-N

Formula: C18H25F3O4

SMILES: CC(OC(=O)CCCC(=O)OCC1=CCC2CC1C2(C)C)C(F)(F)F

Mol. weight [g/mol]: 362.38

Physical Properties

Property code	Value	Unit	Source
gf	-834.66	kJ/mol	Joback Method
hf	-1326.16	kJ/mol	Joback Method
hfus	36.03	kJ/mol	Joback Method
hvap	69.33	kJ/mol	Joback Method
log10ws	-4.77		Crippen Method
logp	4.186		Crippen Method
mcvol	258.650	ml/mol	McGowan Method
pc	1430.46	kPa	Joback Method
rinpol	1887.00		NIST Webbook
rinpol	1887.00		NIST Webbook
tb	775.42	K	Joback Method
tc	968.61	K	Joback Method
tf	491.43	K	Joback Method
vc	1.018	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	818.56	J/mol×K	775.42	Joback Method
cpg	835.43	J/mol×K	807.62	Joback Method
cpg	851.66	J/mol×K	839.82	Joback Method
cpg	867.39	J/mol×K	872.01	Joback Method
cpg	882.72	J/mol×K	904.21	Joback Method
cpg	897.77	J/mol×K	936.41	Joback Method
cpg	912.66	J/mol×K	968.61	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405535&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