Glutaric acid, 1,1,1-trifluoroprop-2-yl 2,4-dimethylpent-3-yl ester

Inchi: InChI=1S/C15H25F3O4/c1-9(2)14(10(3)4)22-13(20)8-6-7-12(19)21-11(5)15(16,17)18/h9-
InchiKey: KGNIRPANTVALEA-UHFFFAOYSA-N
Formula: C15H25F3O4
SMILES: CC(C)C(OC(=O)CCCC(=O)OC(C)C(F)(F)F)C(C)C
Mol. weight [g/mol]: 326.35

Physical Properties

Property code	Value	Unit	Source
gf	-983.77	kJ/mol	Joback Method
hf	-1460.73	kJ/mol	Joback Method
hfus	27.91	kJ/mol	Joback Method
hvap	62.00	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	3.875		Crippen Method
mcvol	242.400	ml/mol	McGowan Method
pc	1423.99	kPa	Joback Method
rinpol	1492.00		NIST Webbook
rinpol	1492.00		NIST Webbook
tb	688.00	K	Joback Method
tc	863.04	K	Joback Method
tf	347.32	K	Joback Method
vc	0.943	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	705.05	J/mol×K	688.00	Joback Method
cpg	720.84	J/mol×K	717.17	Joback Method
cpg	735.78	J/mol×K	746.35	Joback Method
cpg	749.91	J/mol×K	775.52	Joback Method
cpg	763.23	J/mol×K	804.70	Joback Method
cpg	775.76	J/mol×K	833.87	Joback Method
cpg	787.52	J/mol×K	863.04	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393469&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

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