Glutaric acid, 3,5-dimethylcyclohexyl 2,2,3,3-tetrafluoropropyl ester

Inchi: InChI=1S/C16H24F4O4/c1-10-6-11(2)8-12(7-10)24-14(22)5-3-4-13(21)23-9-16(19,20)15

InchiKey: AWBIDUXXHIVNEX-UHFFFAOYSA-N

Formula: C16H24F4O4

SMILES: CC1CC(C)CC(OC(=O)CCCC(=O)OCC(F)(F)C(F)F)C1

Mol. weight [g/mol]: 356.35

Physical Properties

Property code	Value	Unit	Source
gf	-1153.81	kJ/mol	Joback Method
hf	-1648.00	kJ/mol	Joback Method
hfus	38.13	kJ/mol	Joback Method
hvap	64.38	kJ/mol	Joback Method
log10ws	-4.40		Crippen Method
logp	3.968		Crippen Method
mcvol	247.400	ml/mol	McGowan Method
pc	1396.46	kPa	Joback Method
rinpol	1781.00		NIST Webbook
rinpol	1781.00		NIST Webbook
tb	721.68	K	Joback Method
tc	903.70	K	Joback Method
tf	403.08	K	Joback Method
vc	0.966	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	767.03	J/mol×K	721.68	Joback Method
cpg	784.44	J/mol×K	752.02	Joback Method
cpg	800.79	J/mol×K	782.35	Joback Method
cpg	816.10	J/mol×K	812.69	Joback Method
cpg	830.38	J/mol×K	843.03	Joback Method
cpg	843.65	J/mol×K	873.37	Joback Method
cpg	855.93	J/mol×K	903.70	Joback Method

Sources

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=U405406&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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