Glutaric acid, 2,2,3,3-tetrafluoropropyl 3,7-dimethyloctyl ester

Inchi: InChI=1S/C18H30F4O4/c1-13(2)6-4-7-14(3)10-11-25-15(23)8-5-9-16(24)26-12-18(21,22

InchiKey: CXWUTZQIIXZPNF-UHFFFAOYSA-N

Formula: C18H30F4O4

SMILES: CC(C)CCCC(C)CCOC(=O)CCCC(=O)OCC(F)(F)C(F)F

Mol. weight [g/mol]: 386.42

Physical Properties

Property code	Value	Unit	Source
gf	-1150.88	kJ/mol	Joback Method
hf	-1713.48	kJ/mol	Joback Method
hfus	42.29	kJ/mol	Joback Method
hvap	68.25	kJ/mol	Joback Method
log10ws	-5.23		Crippen Method
logp	4.996		Crippen Method
mcvol	286.440	ml/mol	McGowan Method
pc	1117.81	kPa	Joback Method
rinpol	1935.00		NIST Webbook
rinpol	1935.00		NIST Webbook
tb	756.35	K	Joback Method
tc	930.11	K	Joback Method
tf	396.72	K	Joback Method
vc	1.135	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	882.93	J/mol×K	756.35	Joback Method
cpg	899.38	J/mol×K	785.31	Joback Method
cpg	914.92	J/mol×K	814.27	Joback Method
cpg	929.56	J/mol×K	843.23	Joback Method
cpg	943.33	J/mol×K	872.19	Joback Method
cpg	956.26	J/mol×K	901.15	Joback Method
cpg	968.37	J/mol×K	930.11	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391480&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