Glutaric acid, 2,2,3,3-tetrafluoropropyl 4-methylpent-2-yl ester

Inchi: InChI=1S/C14H22F4O4/c1-9(2)7-10(3)22-12(20)6-4-5-11(19)21-8-14(17,18)13(15)16/h9-
InchiKey: HFAHCSCKTJZXNQ-UHFFFAOYSA-N
Formula: C14H22F4O4
SMILES: CC(C)CC(C)OC(=O)CCCC(=O)OCC(F)(F)C(F)F
Mol. weight [g/mol]: 330.32

Physical Properties

Property code	Value	Unit	Source
gf	-1184.56	kJ/mol	Joback Method
hf	-1630.92	kJ/mol	Joback Method
hfus	31.93	kJ/mol	Joback Method
hvap	59.34	kJ/mol	Joback Method
log10ws	-3.91		Crippen Method
logp	3.578		Crippen Method
mcvol	230.080	ml/mol	McGowan Method
pc	1471.36	kPa	Joback Method
rinpol	1506.00		NIST Webbook
rinpol	1506.00		NIST Webbook
tb	664.83	K	Joback Method
tc	832.74	K	Joback Method
tf	351.64	K	Joback Method
vc	0.910	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	657.82	J/mol×K	664.83	Joback Method
cpg	672.49	J/mol×K	692.81	Joback Method
cpg	686.40	J/mol×K	720.80	Joback Method
cpg	699.60	J/mol×K	748.78	Joback Method
cpg	712.07	J/mol×K	776.77	Joback Method
cpg	723.86	J/mol×K	804.75	Joback Method
cpg	734.96	J/mol×K	832.74	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392480&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

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