

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

Inchi: InChI=1S/C15H24F4O4/c1-9(2)13(10(3)4)23-12(21)7-5-6-11(20)22-8-15(18,19)14(16)17
InchiKey: NVCFPFOVYNCPMP-UHFFFAOYSA-N
Formula: C15H24F4O4
SMILES: CC(C)C(OC(=O)CCCC(=O)OCC(F)(F)C(F)F)C(C)C
Mol. weight [g/mol]: 344.34

Physical Properties

Property code	Value	Unit	Source
gf	-1178.58	kJ/mol	Joback Method
hf	-1656.84	kJ/mol	Joback Method
hfus	30.99	kJ/mol	Joback Method
hvap	61.18	kJ/mol	Joback Method
log10ws	-4.08		Crippen Method
logp	3.824		Crippen Method
mvol	244.170	ml/mol	McGowan Method
pc	1376.84	kPa	Joback Method
rinpol	1584.00		NIST Webbook
rinpol	1584.00		NIST Webbook
tb	687.27	K	Joback Method
tc	857.61	K	Joback Method
tf	347.91	K	Joback Method
vc	0.961	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	712.90	J/molxK	687.27	Joback Method
cpg	728.21	J/molxK	715.66	Joback Method
cpg	742.72	J/molxK	744.05	Joback Method
cpg	756.44	J/molxK	772.44	Joback Method
cpg	769.39	J/molxK	800.83	Joback Method
cpg	781.59	J/molxK	829.22	Joback Method
cpg	793.05	J/molxK	857.61	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393470&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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