

Glutaric acid, 2,2,2-trifluoroethyl 2-methylhex-3-yl ester

Inchi:	InChI=1S/C14H23F3O4/c1-4-6-11(10(2)3)21-13(19)8-5-7-12(18)20-9-14(15,16)17/h10-1
InchiKey:	JQWJYMWLZXJVSU-UHFFFAOYSA-N
Formula:	C14H23F3O4
SMILES:	CCCC(OC(=O)CCCC(=O)OCC(F)(F)F)C(C)C
Mol. weight [g/mol]:	312.33

Physical Properties

Property code	Value	Unit	Source
gf	-987.31	kJ/mol	Joback Method
hf	-1429.53	kJ/mol	Joback Method
hfus	32.37	kJ/mol	Joback Method
hvap	60.55	kJ/mol	Joback Method
log10ws	-3.94		Crippen Method
logp	3.630		Crippen Method
mvol	228.310	ml/mol	McGowan Method
pc	1514.03	kPa	Joback Method
rinpol	1481.00		NIST Webbook
rinpol	1481.00		NIST Webbook
tb	666.00	K	Joback Method
tc	836.73	K	Joback Method
tf	366.05	K	Joback Method
vc	0.898	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	649.44	J/molxK	666.00	Joback Method
cpg	664.37	J/molxK	694.46	Joback Method
cpg	678.54	J/molxK	722.91	Joback Method
cpg	691.97	J/molxK	751.37	Joback Method
cpg	704.68	J/molxK	779.82	Joback Method
cpg	716.69	J/molxK	808.28	Joback Method
cpg	728.00	J/molxK	836.73	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380512&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.cheméo.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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