

Glutaric acid, 2,2,3,3-tetrafluoropropyl 3-methylbutyl ester

Inchi:	InChI=1S/C13H20F4O4/c1-9(2)6-7-20-10(18)4-3-5-11(19)21-8-13(16,17)12(14)15/h9,12
InchiKey:	RJAKOBHLEZOMLJ-UHFFFAOYSA-N
Formula:	C13H20F4O4
SMILES:	CC(C)CCOC(=O)CCCC(=O)OCC(F)(F)C(F)F
Mol. weight [g/mol]:	316.29

Physical Properties

Property code	Value	Unit	Source
gf	-1190.54	kJ/mol	Joback Method
hf	-1605.00	kJ/mol	Joback Method
hfus	32.86	kJ/mol	Joback Method
hvap	57.50	kJ/mol	Joback Method
log10ws	-3.38		Crippen Method
logp	3.190		Crippen Method
mcvol	215.990	ml/mol	McGowan Method
pc	1575.95	kPa	Joback Method
rinpol	1611.00		NIST Webbook
rinpol	1611.00		NIST Webbook
tb	642.39	K	Joback Method
tc	807.96	K	Joback Method
tf	355.37	K	Joback Method
vc	0.861	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	604.03	J/mol×K	642.39	Joback Method
cpg	617.98	J/mol×K	669.98	Joback Method
cpg	631.26	J/mol×K	697.58	Joback Method
cpg	643.86	J/mol×K	725.17	Joback Method
cpg	655.81	J/mol×K	752.77	Joback Method
cpg	667.12	J/mol×K	780.36	Joback Method
cpg	677.80	J/mol×K	807.96	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391435&Units=SI

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

Latest version available from:

<https://www.cheméo.com/cid/119-419-5/Glutaric-acid-2-2-3-3-tetrafluoropropyl-3-methylbutyl-ester.pdf>

Generated by Cheméo on 2024-05-04 03:40:12.582329764 +0000 UTC m=+17083261.502907076.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.