

Glutaric acid, 1,1,1-trifluoroprop-2-yl isobutyl ester

Inchi:	InChI=1S/C12H19F3O4/c1-8(2)7-18-10(16)5-4-6-11(17)19-9(3)12(13,14)15/h8-9H,4-7H2
InchiKey:	BJCYAUSWUQJPTF-UHFFFAOYSA-N
Formula:	C12H19F3O4
SMILES:	CC(C)COC(=O)CCCC(=O)OC(C)C(F)(F)F
Mol. weight [g/mol]:	284.27

Physical Properties

Property code	Value	Unit	Source
gf	-1004.15	kJ/mol	Joback Method
hf	-1388.25	kJ/mol	Joback Method
hfus	27.19	kJ/mol	Joback Method
hvap	56.09	kJ/mol	Joback Method
log10ws	-3.10		Crippen Method
logp	2.850		Crippen Method
mvol	200.130	ml/mol	McGowan Method
pc	1768.38	kPa	Joback Method
rinpol	1343.00		NIST Webbook
rinpol	1343.00		NIST Webbook
tb	620.24	K	Joback Method
tc	791.52	K	Joback Method
tf	343.51	K	Joback Method
vc	0.786	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	543.97	J/molxK	620.24	Joback Method
cpg	557.89	J/molxK	648.79	Joback Method
cpg	571.12	J/molxK	677.33	Joback Method
cpg	583.69	J/molxK	705.88	Joback Method
cpg	595.59	J/molxK	734.42	Joback Method
cpg	606.86	J/molxK	762.97	Joback Method
cpg	617.49	J/molxK	791.52	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391497&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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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