

Glutaric acid, 1,1,1-trifluoroprop-2-yl 2-methylhex-3-yl ester

Inchi:	InChI=1S/C15H25F3O4/c1-5-7-12(10(2)3)22-14(20)9-6-8-13(19)21-11(4)15(16,17)18/h1
InchiKey:	XEGMQPAZNNARTF-UHFFFAOYSA-N
Formula:	C15H25F3O4
SMILES:	CCCC(OC(=O)CCCC(=O)OC(C)C(F)(F)F)C(C)C
Mol. weight [g/mol]:	326.35

Physical Properties

Property code	Value	Unit	Source
gf	-981.33	kJ/mol	Joback Method
hf	-1455.45	kJ/mol	Joback Method
hfus	31.44	kJ/mol	Joback Method
hvap	62.39	kJ/mol	Joback Method
log10ws	-4.47		Crippen Method
logp	4.019		Crippen Method
mcvol	242.400	ml/mol	McGowan Method
pc	1415.44	kPa	Joback Method
rinpol	1512.00		NIST Webbook
rinpol	1512.00		NIST Webbook
tb	688.44	K	Joback Method
tc	861.44	K	Joback Method
tf	362.32	K	Joback Method
vc	0.949	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	704.58	J/mol×K	688.44	Joback Method
cpg	720.16	J/mol×K	717.27	Joback Method
cpg	734.92	J/mol×K	746.11	Joback Method
cpg	748.88	J/mol×K	774.94	Joback Method
cpg	762.07	J/mol×K	803.78	Joback Method
cpg	774.49	J/mol×K	832.61	Joback Method
cpg	786.17	J/mol×K	861.44	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=U393724&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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