Glutaric acid, 3-methylbut-2-en-1-yl 2,2,3,3,3-pentafluoropropyl ester

Inchi: InChI=1S/C13H17F5O4/c1-9(2)6-7-21-10(19)4-3-5-11(20)22-8-12(14,15)13(16,17)18/h6

InchiKey: TWWRGRNGTRAHLJ-UHFFFAOYSA-N

Formula: C13H17F5O4

SMILES: CC(C)=CCOC(=O)CCCC(=O)OCC(F)(F)C(F)(F)F

Mol. weight [g/mol]: 332.26

Physical Properties

Property code	Value	Unit	Source
gf	-1305.96	kJ/mol	Joback Method
hf	-1691.87	kJ/mol	Joback Method
hfus	34.46	kJ/mol	Joback Method
hvap	56.20	kJ/mol	Joback Method
log10ws	-3.82		Crippen Method
logp	3.407		Crippen Method
mcvol	213.460	ml/mol	McGowan Method
pc	1594.89	kPa	Joback Method
rinpol	1413.00		NIST Webbook
rinpol	1413.00		NIST Webbook
tb	643.35	K	Joback Method
tc	812.05	K	Joback Method
tf	369.34	K	Joback Method
vc	0.861	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	592.49	J/mol×K	643.35	Joback Method
cpg	605.53	J/mol×K	671.47	Joback Method
cpg	617.84	J/mol×K	699.58	Joback Method
cpg	629.46	J/mol×K	727.70	Joback Method
cpg	640.42	J/mol×K	755.82	Joback Method
cpg	650.75	J/mol×K	783.94	Joback Method
cpg	660.48	J/mol×K	812.05	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393668&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
hvap:	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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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