Glutaric acid, dec-2-yl 2,2,3,3,3-pentafluoropropyl ester

Inchi: InChI=1S/C18H29F5O4/c1-3-4-5-6-7-8-10-14(2)27-16(25)12-9-11-15(24)26-13-17(19,20)18(21,22)23

InchiKey: JTWCBEYEUSKHAB-UHFFFAOYSA-N

Formula: C18H29F5O4

SMILES: CCCCCCCCC(C)OC(=O)CCCC(=O)OCC(F)(F)C(F)(F)F

Mol. weight [g/mol]: 404.41

Physical Properties

Property code	Value	Unit	Source
gf	-1337.97	kJ/mol	Joback Method
hf	-1907.78	kJ/mol	Joback Method
hfus	45.00	kJ/mol	Joback Method
hvap	66.91	kJ/mol	Joback Method
log10ws	-6.17		Crippen Method
logp	5.580		Crippen Method
mcvol	288.210	ml/mol	McGowan Method
pc	1087.06	kPa	Joback Method
rinpol	1778.00		NIST Webbook
rinpol	1778.00		NIST Webbook
tb	753.27	K	Joback Method
tc	925.22	K	Joback Method
tf	429.73	K	Joback Method
vc	1.153	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	891.25	J/mol×K	753.27	Joback Method
cpg	907.22	J/mol×K	781.93	Joback Method
cpg	922.28	J/mol×K	810.59	Joback Method
cpg	936.49	J/mol×K	839.24	Joback Method
cpg	949.87	J/mol×K	867.90	Joback Method
cpg	962.46	J/mol×K	896.56	Joback Method
cpg	974.28	J/mol×K	925.22	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393677&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
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