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

Inchi: InChI=1S/C16H15F5O4/c1-8(2)6-7-24-9(22)4-3-5-10(23)25-16-14(20)12(18)11(17)13(19

InchiKey: GYDJVQZQMLHPHN-UHFFFAOYSA-N

Formula: C16H15F5O4

SMILES: CC(C)=CCOC(=O)CCCC(=O)Oc1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 366.28

Physical Properties

Property code	Value	Unit	Source
gf	-1222.12	kJ/mol	Joback Method
hf	-1557.11	kJ/mol	Joback Method
hfus	49.16	kJ/mol	Joback Method
hvap	71.06	kJ/mol	Joback Method
log10ws	-5.51		Crippen Method
logp	3.967		Crippen Method
mcvol	231.970	ml/mol	McGowan Method
pc	1509.33	kPa	Joback Method
rinpol	1836.00		NIST Webbook
rinpol	1836.00		NIST Webbook
tb	770.03	K	Joback Method
tc	955.19	K	Joback Method
tf	487.33	K	Joback Method
vc	0.943	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	658.07	J/mol×K	770.03	Joback Method
cpg	670.11	J/mol×K	800.89	Joback Method
cpg	681.42	J/mol×K	831.75	Joback Method
cpg	692.01	J/mol×K	862.61	Joback Method
cpg	701.89	J/mol×K	893.47	Joback Method
cpg	711.06	J/mol×K	924.33	Joback Method
cpg	719.53	J/mol×K	955.19	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=U392108&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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