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

Inchi: InChI=1S/C17H17F5O4/c1-9(2)6-7-25-11(23)4-3-5-12(24)26-8-10-13(18)15(20)17(22)16

InchiKey: OVEWEPQOJMWZBS-UHFFFAOYSA-N

Formula: C17H17F5O4

SMILES: CC(C)=CCOC(=O)CCCC(=O)OCc1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 380.31

Physical Properties

Property code	Value	Unit	Source
gf	-1213.70	kJ/mol	Joback Method
hf	-1577.75	kJ/mol	Joback Method
hfus	51.75	kJ/mol	Joback Method
hvap	73.29	kJ/mol	Joback Method
log10ws	-5.77		Crippen Method
logp	4.105		Crippen Method
mcvol	246.060	ml/mol	McGowan Method
pc	1402.74	kPa	Joback Method
rinpol	1998.00		NIST Webbook
rinpol	1998.00		NIST Webbook
tb	792.91	K	Joback Method
tc	979.26	K	Joback Method
tf	498.60	K	Joback Method
vc	0.999	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	713.21	J/mol×K	792.91	Joback Method
cpg	725.73	J/mol×K	823.97	Joback Method
cpg	737.46	J/mol×K	855.03	Joback Method
cpg	748.43	J/mol×K	886.09	Joback Method
cpg	758.63	J/mol×K	917.15	Joback Method
cpg	768.08	J/mol×K	948.21	Joback Method
cpg	776.79	J/mol×K	979.26	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=U391930&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