2-(4-Methylcyclohex-3-enyl)propan-2-yl 2,3,4,5,6-pentafluorobenzoate

Inchi: InChI=1S/C17H17F5O2/c1-8-4-6-9(7-5-8)17(2,3)24-16(23)10-11(18)13(20)15(22)14(21)1

InchiKey: JCBVATYWTBSVOR-UHFFFAOYSA-N

Formula: C17H17F5O2

SMILES: CC1=CCC(C(C)(C)OC(=O)c2c(F)c(F)c(F)c(F)c2F)CC1

Mol. weight [g/mol]: 348.31

Physical Properties

Property code	Value	Unit	Source
gf	-1003.83	kJ/mol	Joback Method
hf	-1348.50	kJ/mol	Joback Method
hfus	35.32	kJ/mol	Joback Method
hvap	64.18	kJ/mol	Joback Method
log10ws	-6.76		Crippen Method
logp	5.064		Crippen Method
mcvol	227.760	ml/mol	McGowan Method
pc	1564.75	kPa	Joback Method
rinpol	1789.00		NIST Webbook
tb	733.04	K	Joback Method
tc	931.46	K	Joback Method
tf	468.56	K	Joback Method
vc	0.901	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	662.53	J/mol×K	733.04	Joback Method
cpg	677.64	J/mol×K	766.11	Joback Method
cpg	691.77	J/mol×K	799.18	Joback Method
cpg	704.93	J/mol×K	832.25	Joback Method
cpg	717.14	J/mol×K	865.32	Joback Method
cpg	728.45	J/mol×K	898.39	Joback Method
cpg	738.86	J/mol×K	931.46	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373596&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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