Decan-2-yl 2,3,4,5,6-pentafluorobenzoate

Inchi: InChI=1S/C17H21F5O2/c1-3-4-5-6-7-8-9-10(2)24-17(23)11-12(18)14(20)16(22)15(21)13
InchiKey: RMOYAZMJLBETSH-UHFFFAOYSA-N
Formula: C17H21F5O2
SMILES: CCCCCCCCC(C)OC(=O)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 352.34

Physical Properties

Property code	Value	Unit	Source
gf	-1053.89	kJ/mol	Joback Method
hf	-1445.66	kJ/mol	Joback Method
hfus	46.55	kJ/mol	Joback Method
hvap	63.70	kJ/mol	Joback Method
log10ws	-7.25		Crippen Method
logp	5.678		Crippen Method
mcvol	242.920	ml/mol	McGowan Method
pc	1308.01	kPa	Joback Method
rinpol	1745.00		NIST Webbook
rinpol	1745.00		NIST Webbook
tb	712.14	K	Joback Method
tc	884.85	K	Joback Method
tf	430.48	K	Joback Method
vc	0.988	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	692.66	J/mol×K	712.14	Joback Method
cpg	707.10	J/mol×K	740.92	Joback Method
cpg	720.83	J/mol×K	769.71	Joback Method
cpg	733.86	J/mol×K	798.49	Joback Method
cpg	746.19	J/mol×K	827.28	Joback Method
cpg	757.84	J/mol×K	856.06	Joback Method
cpg	768.80	J/mol×K	884.85	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373594&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