3-Heptafluorobutyryloxy-4-methoxybenzyl alcohol, O-pentafluoropropionyl-

Inchi: InChI=1S/C15H8F12O5/c1-30-7-3-2-6(5-31-9(28)12(18,19)14(22,23)24)4-8(7)32-10(29)1

InchiKey: NZHYSFOYCDBYFI-UHFFFAOYSA-N

Formula: C15H8F12O5

SMILES: COc1ccc(COC(=O)C(F)(F)C(F)(F)F)cc1OC(=O)C(F)(F)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 496.20

Physical Properties

Property code	Value	Unit	Source
gf	-2727.79	kJ/mol	Joback Method
hf	-3158.23	kJ/mol	Joback Method
hfus	34.52	kJ/mol	Joback Method
hvap	57.02	kJ/mol	Joback Method
log10ws	-6.01		Crippen Method
logp	4.674		Crippen Method
mcvol	240.440	ml/mol	McGowan Method
pc	1344.71	kPa	Joback Method
rinpol	1409.00		NIST Webbook
rinpol	1409.00		NIST Webbook
tb	729.33	K	Joback Method
tc	901.63	K	Joback Method
tf	496.00	K	Joback Method
vc	0.995	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	725.51	J/mol×K	729.33	Joback Method
cpg	735.67	J/mol×K	758.05	Joback Method
cpg	745.01	J/mol×K	786.76	Joback Method
cpg	753.60	J/mol×K	815.48	Joback Method
cpg	761.48	J/mol×K	844.20	Joback Method
cpg	768.71	J/mol×K	872.91	Joback Method
cpg	775.34	J/mol×K	901.63	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=U374852&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