Methyl 3-heptafluorobutyryloxybenzoate

Inchi: InChI=1S/C12H7F7O4/c1-22-8(20)6-3-2-4-7(5-6)23-9(21)10(13,14)11(15,16)12(17,18)19
InchiKey: LCJHNYQPDKTTJI-UHFFFAOYSA-N
Formula: C12H7F7O4
SMILES: COC(=O)c1cccc(OC(=O)C(F)(F)C(F)(F)C(F)(F)F)c1
Mol. weight [g/mol]: 348.17

Physical Properties

Property code	Value	Unit	Source
gf	-1670.05	kJ/mol	Joback Method
hf	-1954.57	kJ/mol	Joback Method
hfus	25.38	kJ/mol	Joback Method
hvap	53.95	kJ/mol	Joback Method
log10ws	-4.16		Crippen Method
logp	3.211		Crippen Method
mcvol	183.450	ml/mol	McGowan Method
pc	2029.06	kPa	Joback Method
rinpol	1293.00		NIST Webbook
rinpol	1293.00		NIST Webbook
tb	643.40	K	Joback Method
tc	828.09	K	Joback Method
tf	419.65	K	Joback Method
vc	0.741	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	502.86	J/mol×K	643.40	Joback Method
cpg	513.65	J/mol×K	674.18	Joback Method
cpg	523.62	J/mol×K	704.96	Joback Method
cpg	532.79	J/mol×K	735.75	Joback Method
cpg	541.23	J/mol×K	766.53	Joback Method
cpg	548.97	J/mol×K	797.31	Joback Method
cpg	556.06	J/mol×K	828.09	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374623&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

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