2,4,5-Trifluoro-3-methoxybenzoic acid, cyclohexylmethyl ester

Inchi: InChI=1S/C15H17F3O3/c1-20-14-12(17)10(7-11(16)13(14)18)15(19)21-8-9-5-3-2-4-6-9/h

InchiKey: COWLDMAWAGENJZ-UHFFFAOYSA-N

Formula: C15H17F3O3

SMILES: COc1c(F)c(F)cc(C(=O)OCC2CCCCC2)c1F

Mol. weight [g/mol]: 302.29

Physical Properties

Property code	Value	Unit	Source
gf	-749.59	kJ/mol	Joback Method
hf	-1073.31	kJ/mol	Joback Method
hfus	32.14	kJ/mol	Joback Method
hvap	63.45	kJ/mol	Joback Method
log10ws	-4.99		Crippen Method
logp	3.850		Crippen Method
mcvol	206.210	ml/mol	McGowan Method
pc	1910.24	kPa	Joback Method
rinpol	1925.00		NIST Webbook
rinpol	1925.00		NIST Webbook
tb	705.27	K	Joback Method
tc	909.18	K	Joback Method
tf	438.85	K	Joback Method
vc	0.796	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	589.08	J/mol×K	705.27	Joback Method
cpg	605.19	J/mol×K	739.26	Joback Method
cpg	620.28	J/mol×K	773.24	Joback Method
cpg	634.35	J/mol×K	807.23	Joback Method
cpg	647.40	J/mol×K	841.21	Joback Method
cpg	659.42	J/mol×K	875.20	Joback Method
cpg	670.42	J/mol×K	909.18	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=U357613&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