Cyclobutanecarboxylic acid, 3,5-difluorophenyl ester

Inchi: InChI=1S/C11H10F2O2/c12-8-4-9(13)6-10(5-8)15-11(14)7-2-1-3-7/h4-7H,1-3H2

InchiKey: XWXGISDKVLWMRR-UHFFFAOYSA-N

Formula: C11H10F2O2

SMILES: O=C(Oc1cc(F)cc(F)c1)C1CCC1

Mol. weight [g/mol]: 212.19

Physical Properties

Property code	Value	Unit	Source
gf	-440.00	kJ/mol	Joback Method
hf	-627.16	kJ/mol	Joback Method
hfus	22.49	kJ/mol	Joback Method
hvap	51.29	kJ/mol	Joback Method
log10ws	-3.36		Crippen Method
logp	2.670		Crippen Method
mcvol	142.210	ml/mol	McGowan Method
pc	2884.30	kPa	Joback Method
rinpol	1329.00		NIST Webbook
tb	573.56	K	Joback Method
tc	786.44	K	Joback Method
tf	352.95	K	Joback Method
vc	0.552	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	348.26	J/mol×K	573.56	Joback Method
cpg	362.22	J/mol×K	609.04	Joback Method
cpg	375.31	J/mol×K	644.52	Joback Method
cpg	387.57	J/mol×K	680.00	Joback Method
cpg	399.03	J/mol×K	715.48	Joback Method
cpg	409.71	J/mol×K	750.96	Joback Method
cpg	419.64	J/mol×K	786.44	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=U299070&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