Cyclobutanecarboxylic acid, 2-bromo-4-fluorophenyl ester

Inchi: InChI=1S/C11H10BrFO2/c12-9-6-8(13)4-5-10(9)15-11(14)7-2-1-3-7/h4-7H,1-3H2

InchiKey: OIZOYTFBIHYZBY-UHFFFAOYSA-N

Formula: C11H10BrFO2

SMILES: O=C(Oc1ccc(F)cc1Br)C1CCC1

Mol. weight [g/mol]: 273.10

Physical Properties

Property code	Value	Unit	Source
gf	-230.87	kJ/mol	Joback Method
hf	-404.72	kJ/mol	Joback Method
hfus	24.70	kJ/mol	Joback Method
hvap	58.54	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	3.294		Crippen Method
mcvol	157.940	ml/mol	McGowan Method
pc	3272.78	kPa	Joback Method
rinpol	1572.00		NIST Webbook
tb	640.45	K	Joback Method
tc	876.60	K	Joback Method
tf	412.16	K	Joback Method
vc	0.597	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	377.79	J/mol×K	640.45	Joback Method
cpg	391.09	J/mol×K	679.81	Joback Method
cpg	403.41	J/mol×K	719.17	Joback Method
cpg	414.81	J/mol×K	758.53	Joback Method
cpg	425.32	J/mol×K	797.88	Joback Method
cpg	435.01	J/mol×K	837.24	Joback Method
cpg	443.92	J/mol×K	876.60	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=U299074&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