2C-B-FLY TFA

Inchi: InChI=1S/C14H13BrF3NO3/c15-10-9-3-6-21-11(9)7(8-2-5-22-12(8)10)1-4-19-13(20)14(1
InchiKey: LHOPHBFOOLNLLJ-UHFFFAOYSA-N
Formula: C14H13BrF3NO3
SMILES: O=C(NCCc1c2c(c(Br)c3c1OCC3)OCC2)C(F)(F)F
Mol. weight [g/mol]: 380.16

Physical Properties

Property code	Value	Unit	Source
hfus	48.01	kJ/mol	Joback Method
logp	2.540		Crippen Method
mcvol	208.740	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	600.40	J/mol×K	812.80	Joback Method
cpg	611.30	J/mol×K	849.91	Joback Method
cpg	621.62	J/mol×K	887.03	Joback Method
cpg	631.48	J/mol×K	924.14	Joback Method
cpg	641.00	J/mol×K	961.26	Joback Method
cpg	650.33	J/mol×K	998.37	Joback Method
cpg	659.58	J/mol×K	1035.49	Joback Method

Sources

Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R640476&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume