

Bisphenol AF

Inchi: InChI=1S/C15H10F6O2/c16-14(17,18)13(15(19,20)21,9-1-5-11(22)6-2-9)10-3-7-12(23)8

InchiKey: ZFVMWEVVKGLCIJ-UHFFFAOYSA-N

Formula: C15H10F6O2

SMILES: Oc1ccc(C(c2ccc(O)cc2)(C(F)(F)F)C(F)(F)F)cc1

Mol. weight [g/mol]: 336.23

CAS: 1478-61-1

Physical Properties

Property code	Value	Unit	Source
hf	-1419.56	kJ/mol	Cheméo Relay (1.0)
hfus	30.49	kJ/mol	Joback Method
hvap	103.53	kJ/mol	Cheméo Relay (1.0)
ie	8.62	eV	Cheméo Relay (1.0)
log10ws	-4.82		Cheméo Relay (1.0)
logp	4.509		Crippen Method
mcvol	197.050	ml/mol	McGowan Method
tb	591.14	K	Cheméo Relay (1.0)
tf	434.15	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	-1.33270e+02
Coeff. B	2.02840e+00
Coeff. C	-1.98112e-03
Coeff. D	7.33800e-07
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00

Sources

Cheméo Relay (1.0, beta):

Jean-Claude Bradley Open Melting
Point Dataset (2014, CC0):
Joback Method:

https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Dataset/1031637

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>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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