BIS(P-FLUOROPHENYL)METHANOL

Other names: Bis-(4-fluorophenyl)-methanol
Benzenemethanol, 4-fluoro-«alpha»-(4-fluorophenyl)-
4,4'-difluorobenzhydryl alcohol
Inchi: InChI=1S/C13H10F2O/c14-11-5-1-9(2-6-11)13(16)10-3-7-12(15)8-4-10/h1-8,13,16H
InchiKey: WCTZPQWLFWZYJE-UHFFFAOYSA-N
Formula: C13H10F2O
SMILES: OC(c1ccc(F)cc1)c1ccc(F)cc1
Mol. weight [g/mol]: 220.22

Physical Properties

Property code	Value	Unit	Source
af	0.6391		Cheméo Relay (1.0)
gf	-264.74	kJ/mol	Joback Method
hf	-381.19	kJ/mol	Cheméo Relay (1.0)
hfus	23.46	kJ/mol	Joback Method
hvap	91.08	kJ/mol	Cheméo Relay (1.0)
ie	8.87	eV	Cheméo Relay (1.0)
log10ws	-2.92		Cheméo Relay (1.0)
logp	3.046		Crippen Method
mcvol	155.920	ml/mol	McGowan Method
pc	3005.73	kPa	Joback Method
tb	528.04	K	Cheméo Relay (1.0)
tc	821.16	K	Cheméo Relay (1.0)
tf	353.48	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	393.24	J/mol×K	650.44	Joback Method
cpg	405.18	J/mol×K	685.47	Joback Method
cpg	416.28	J/mol×K	720.49	Joback Method
cpg	426.60	J/mol×K	755.52	Joback Method
cpg	436.17	J/mol×K	790.55	Joback Method
cpg	445.04	J/mol×K	825.57	Joback Method

cpg	453.25	J/mol×K	860.60	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C365242&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

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

Legend

af: Acentric Factor
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
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point