L-(4-Fluorophenyl)-2-phenylethane

Other names:	Bibenzyl, 4-fluoro- 4-Fluorobibenzyl 1-(4-Fluorophenyl)-2-phenylethane L-(4-Fluorophenyl)-2-phenylethane
Inchi:	InChI=1S/C14H13F/c15-14-10-8-13(9-11-14)7-6-12-4-2-1-3-5-12/h1-5,8-11H,6-7H2
InchiKey:	LGAWAQNSZFCGMP-UHFFFAOYSA-N
Formula:	C14H13F
SMILES:	Fc1ccc(CCc2ccccc2)cc1
Mol. weight [g/mol]:	200.26

Physical Properties

Property code	Value	Unit	Source
af	0.4567		Cheméo Relay (1.0)
gf	87.38	kJ/mol	Joback Method
hf	-49.33	kJ/mol	Cheméo Relay (1.0)
hfus	22.79	kJ/mol	Joback Method
hvap	78.87	kJ/mol	Cheméo Relay (1.0)
ie	8.80 ± 0.10	eV	NIST Webbook
log10ws	-4.55		Cheméo Relay (1.0)
logp	3.611		Crippen Method
mcvol	162.370	ml/mol	McGowan Method
pc	2603.08	kPa	Joback Method
tb	549.39	K	Cheméo Relay (1.0)
tc	778.22	K	Cheméo Relay (1.0)
tf	302.84	K	Cheméo Relay (1.0)
vc	0.618	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	380.31	J/mol×K	577.33	Joback Method
cpg	396.84	J/mol×K	615.42	Joback Method
cpg	412.20	J/mol×K	653.52	Joback Method
cpg	426.45	J/mol×K	691.61	Joback Method

cpg	439.65	J/mol×K	729.71	Joback Method
cpg	451.86	J/mol×K	767.80	Joback Method
cpg	463.15	J/mol×K	805.90	Joback Method

Sources

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):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C370763&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
vc:	Critical Volume