

(2E,4E)-5-(Benzo[d][1,3]dioxol-5-yl)-N-isobutylpen

Inchi:	InChI=1S/C16H19NO3/c1-12(2)10-17-16(18)6-4-3-5-13-7-8-14-15(9-13)20-11-19-14/h3-5
InchiKey:	WHAAPCGHVWVUEX-GGWOSOGESA-N
Formula:	C16H19NO3
SMILES:	CC(C)CNC(=O)C=CC=Cc1ccc2c(c1)OCO2
Mol. weight [g/mol]:	273.33
CAS:	5950-12-9

Physical Properties

Property code	Value	Unit	Source
gf	191.68	kJ/mol	Joback Method
hf	-160.79	kJ/mol	Joback Method
hfus	47.06	kJ/mol	Joback Method
hvap	76.76	kJ/mol	Joback Method
log10ws	-4.01		Crippen Method
logp	2.757		Crippen Method
mcvol	216.370	ml/mol	McGowan Method
pc	2224.99	kPa	Joback Method
rinpol	2626.00		NIST Webbook
rinpol	2626.00		NIST Webbook
rinpol	2667.70		NIST Webbook
rinpol	2667.70		NIST Webbook
tb	779.35	K	Joback Method
tc	1004.73	K	Joback Method
tf	474.29	K	Joback Method
vc	0.819	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	624.52	J/molxK	779.35	Joback Method
cpg	638.72	J/molxK	816.91	Joback Method
cpg	652.04	J/molxK	854.48	Joback Method
cpg	664.62	J/molxK	892.04	Joback Method
cpg	676.55	J/molxK	929.61	Joback Method

cpg	687.95	J/mol×K	967.17	Joback Method
cpg	698.95	J/mol×K	1004.73	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=C5950129&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	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

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