

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

Inchi:	InChI=1S/C16H21NO3/c1-12(2)10-17-16(18)6-4-3-5-13-7-8-14-15(9-13)20-11-19-14/h4,6,10,12,14,16,18,20
InchiKey:	CSGDXLXTJVRNEA-GQCTYLIASA-N
Formula:	C16H21NO3
SMILES:	CC(C)CNC(=O)C=CCCc1ccc2c(c1)OCO2
Mol. weight [g/mol]:	275.34
CAS:	23512-53-0

Physical Properties

Property code	Value	Unit	Source
gf	111.46	kJ/mol	Joback Method
hf	-278.01	kJ/mol	Joback Method
hfus	46.86	kJ/mol	Joback Method
hvap	76.80	kJ/mol	Joback Method
log10ws	-3.99		Crippen Method
logp	2.676		Crippen Method
mcvol	220.670	ml/mol	McGowan Method
pc	2119.73	kPa	Joback Method
rinpol	2410.40		NIST Webbook
rinpol	2387.00		NIST Webbook
rinpol	2387.00		NIST Webbook
rinpol	2410.40		NIST Webbook
tb	775.19	K	Joback Method
tc	993.32	K	Joback Method
tf	479.37	K	Joback Method
vc	0.839	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	649.85	J/molxK	775.19	Joback Method
cpg	664.55	J/molxK	811.55	Joback Method
cpg	678.35	J/molxK	847.90	Joback Method
cpg	691.31	J/molxK	884.26	Joback Method
cpg	703.55	J/molxK	920.61	Joback Method

cpg	715.15	J/mol×K	956.97	Joback Method
cpg	726.19	J/mol×K	993.32	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C23512530&Units=SI

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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