2-(3',4'-Methylenedioxyphenylethyl)-1,2,3,4-tetrahydroquinoline

Inchi: InChI=1S/C18H19NO2/c1-2-4-16-14(3-1)7-9-15(19-16)8-5-13-6-10-17-18(11-13)21-12-2

InchiKey: UTJHHIWJBNBFJH-UHFFFAOYSA-N

Formula: C18H19NO2

SMILES: c1ccc2c(c1)CCC(CCc1ccc3c(c1)OCO3)N2

Mol. weight [g/mol]: 281.35

Physical Properties

Property code	Value	Unit	Source
gf	329.19	kJ/mol	Joback Method
hf	-42.61	kJ/mol	Joback Method
hfus	47.94	kJ/mol	Joback Method
hvap	78.28	kJ/mol	Joback Method
log10ws	-4.95		Crippen Method
logp	3.775		Crippen Method
mcvol	216.960	ml/mol	McGowan Method
pc	2490.03	kPa	Joback Method
tb	804.41	K	Joback Method
tc	1060.21	K	Joback Method
tf	577.79	K	Joback Method
vc	0.814	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	658.05	J/mol×K	804.41	Joback Method
cpg	675.05	J/mol×K	847.04	Joback Method
cpg	690.78	J/mol×K	889.68	Joback Method
cpg	705.39	J/mol×K	932.31	Joback Method
cpg	719.03	J/mol×K	974.95	Joback Method
cpg	731.85	J/mol×K	1017.58	Joback Method
cpg	744.01	J/mol×K	1060.21	Joback Method

Sources

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=R398244&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
hvap:	Enthalpy of vaporization at standard conditions
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