

endo-Arbozyl angelate

Inchi:

InChI=1S/C18H26O2/c1-7-12(4)17(19)20-10-16-8-15-9-18(16,11(2)3)14(6)13(15)5/h7,15

InchiKey:

IYIHUFNVXVJOTK-MEDCJMHOSA-N

Formula:

C18H26O2

SMILES:

C=C(C)C12CC(CC1COC(=O)C(C)=CC)C(C)=C2C

Mol. weight [g/mol]:

274.40

Physical Properties

Property code	Value	Unit	Source
gf	124.62	kJ/mol	Joback Method
hf	-267.40	kJ/mol	Joback Method
hfus	30.85	kJ/mol	Joback Method
hvap	64.42	kJ/mol	Joback Method
log10ws	-4.85		Crippen Method
logp	4.434		Crippen Method
mcvol	237.300	ml/mol	McGowan Method
pc	1609.00	kPa	Joback Method
ripol	2209.00		NIST Webbook
ripol	2209.00		NIST Webbook
tb	710.57	K	Joback Method
tc	921.35	K	Joback Method
tf	407.84	K	Joback Method
vc	0.919	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	690.89	J/mol×K	710.57	Joback Method
cpg	709.89	J/mol×K	745.70	Joback Method
cpg	728.11	J/mol×K	780.83	Joback Method
cpg	745.69	J/mol×K	815.96	Joback Method
cpg	762.81	J/mol×K	851.09	Joback Method
cpg	779.61	J/mol×K	886.22	Joback Method
cpg	796.25	J/mol×K	921.35	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R639713&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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