

«alpha»-Phellandrene dimer

Inchi: InChI=1S/C20H32/c1-11(2)15-8-7-13(5)19-18-9-14(6)17(20(15)19)10-16(18)12(3)4/h7,9,
InchiKey: YCGKKSPKOFEYNJ-UHFFFAOYSA-N
Formula: C20H32
SMILES: CC1=CC2C(C(C)C)CC1C1C(C(C)C)CC=C(C)C21
Mol. weight [g/mol]: 272.47

Physical Properties

Property code	Value	Unit	Source
hfus	33.49	kJ/mol	Joback Method
logp	5.709		Crippen Method
mcvol	251.480	ml/mol	McGowan Method
rinpol	1804.00		NIST Webbook
rinpol	1804.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	770.85	J/mol×K	683.42	Joback Method
cpg	795.58	J/mol×K	718.35	Joback Method
cpg	818.85	J/mol×K	753.27	Joback Method
cpg	840.72	J/mol×K	788.20	Joback Method
cpg	861.27	J/mol×K	823.13	Joback Method
cpg	880.60	J/mol×K	858.06	Joback Method
cpg	898.77	J/mol×K	892.98	Joback Method
dvisc	0.0019197	Pa×s	342.26	Joback Method
dvisc	0.0016770	Pa×s	399.12	Joback Method
dvisc	0.0015152	Pa×s	455.98	Joback Method
dvisc	0.0014001	Pa×s	512.84	Joback Method
dvisc	0.0013144	Pa×s	569.70	Joback Method
dvisc	0.0012481	Pa×s	626.56	Joback Method
dvisc	0.0011954	Pa×s	683.42	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R626014&Units=SI>

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

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
dvisc:	Dynamic viscosity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpola:	Non-polar retention indices

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