«alpha»-Calamenene

Inchi: InChI=1S/C15H22/c1-10(2)13-8-6-12(4)14-7-5-11(3)9-15(13)14/h5,7,9-10,12-13H,6,8H2,
InchiKey: PGTJIOWQJWHTJJ-STQMWFEESA-N
Formula: C15H22
SMILES: Cc1ccc2c(c1)C(C(C)C)CCC2C
Mol. weight [g/mol]: 202.34

Physical Properties

Property code	Value	Unit	Source
hfus	21.45	kJ/mol	Joback Method
ie	7.92	eV	Cheméo Relay (1.0)
logp	4.632		Crippen Method
mcvol	187.590	ml/mol	McGowan Method
rinpol	1498.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	482.92	J/mol×K	585.14	Joback Method
cpg	503.81	J/mol×K	621.55	Joback Method
cpg	523.46	J/mol×K	657.97	Joback Method
cpg	541.93	J/mol×K	694.38	Joback Method
cpg	559.26	J/mol×K	730.80	Joback Method
cpg	575.50	J/mol×K	767.21	Joback Method
cpg	590.72	J/mol×K	803.63	Joback Method
dvisc	0.0018212	Pa×s	305.45	Joback Method
dvisc	0.0011104	Pa×s	352.07	Joback Method
dvisc	0.0007601	Pa×s	398.68	Joback Method
dvisc	0.0005632	Pa×s	445.30	Joback Method
dvisc	0.0004418	Pa×s	491.91	Joback Method
dvisc	0.0003614	Pa×s	538.53	Joback Method
dvisc	0.0003052	Pa×s	585.14	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R620987&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

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices