«gamma»-Pyronene

Inchi: InChI=1S/C10H16/c1-8-5-9(2)7-10(3,4)6-8/h5-6H,7H2,1-4H3
InchiKey: SZHAWDAGEJWQJK-UHFFFAOYSA-N
Formula: C10H16
SMILES: CC1=CC(C)(C)CC(C)=C1
Mol. weight [g/mol]: 136.23

Physical Properties

Property code	Value	Unit	Source
hfus	8.86	kJ/mol	Joback Method
logp	3.309		Crippen Method
mcvol	132.300	ml/mol	McGowan Method
rinpol	1345.00		NIST Webbook
rinpol	1345.00		NIST Webbook
rinpol	1345.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	273.78	J/mol×K	456.27	Joback Method
cpg	290.27	J/mol×K	491.70	Joback Method
cpg	305.70	J/mol×K	527.12	Joback Method
cpg	320.17	J/mol×K	562.55	Joback Method
cpg	333.78	J/mol×K	597.98	Joback Method
cpg	346.62	J/mol×K	633.40	Joback Method
cpg	358.81	J/mol×K	668.83	Joback Method

Sources

Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R615613&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
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices