iso-«beta»-terpineol

Inchi: InChI=1S/C10H18O/c1-8(2)9-4-6-10(3,11)7-5-9/h9,11H,1,4-7H2,2-3H3
InchiKey: RUJPNZNXGCHGID-UHFFFAOYSA-N
Formula: C10H18O
SMILES: C=C(C)C1CCC(C)(O)CC1
Mol. weight [g/mol]: 154.25

Physical Properties

Property code	Value	Unit	Source
hfus	9.76	kJ/mol	Joback Method
ie	9.00	eV	Cheméo Relay (1.0)
logp	2.504		Crippen Method
mcvol	142.470	ml/mol	McGowan Method
ripol	1437.00		NIST Webbook
ripol	1437.00		NIST Webbook
tb	490.53	K	Cheméo Relay (1.0)
tf	291.71	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	349.49	J/mol×K	532.06	Joback Method
cpg	365.75	J/mol×K	565.47	Joback Method
cpg	381.06	J/mol×K	598.89	Joback Method
cpg	395.50	J/mol×K	632.30	Joback Method
cpg	409.18	J/mol×K	665.71	Joback Method
cpg	422.18	J/mol×K	699.12	Joback Method
cpg	434.60	J/mol×K	732.54	Joback Method

Sources

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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R313887&Units=SI

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point