Tricyclo[2.2.1.0(2,6)]heptan-3-ol, 4,5,5-trimethyl-

Other names: «beta»-Pericyclocamphanol
Inchi: InChI=1S/C10H16O/c1-9(2)7-5-4-10(9,3)8(11)6(5)7/h5-8,11H,4H2,1-3H3
InchiKey: DVHLXMZZPWNOGD-UHFFFAOYSA-N
Formula: C10H16O
SMILES: CC1(C)C2C3CC1(C)C(O)C32
Mol. weight [g/mol]: 152.23
CAS: 62560-53-6

Physical Properties

Property code	Value	Unit	Source
gf	68.84	kJ/mol	Joback Method
hf	-201.78	kJ/mol	Joback Method
hfus	14.97	kJ/mol	Joback Method
hvap	50.70	kJ/mol	Joback Method
log10ws	-1.86		Crippen Method
logp	1.659		Crippen Method
mcvol	125.050	ml/mol	McGowan Method
pc	3246.73	kPa	Joback Method
rinpol	1149.00		NIST Webbook
rinpol	1149.00		NIST Webbook
tb	518.53	K	Joback Method
tc	712.79	K	Joback Method
tf	359.22	K	Joback Method
vc	0.494	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	340.10	J/mol×K	518.53	Joback Method
cpg	354.82	J/mol×K	550.91	Joback Method
cpg	368.35	J/mol×K	583.28	Joback Method
cpg	380.87	J/mol×K	615.66	Joback Method
cpg	392.59	J/mol×K	648.04	Joback Method
cpg	403.72	J/mol×K	680.41	Joback Method

cpg	414.46	J/mol×K	712.79	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C62560536&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:
https://www.chemeo.com/cid/79-678-3/Tricyclo-2-2-1-0-2-6-heptan-3-ol-4-5-5-trimethyl.pdf
Generated by Cheméo on 2024-04-30 01:01:12.265403138 +0000 UTC m=+16728121.185980451.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.