2,4,6-Trimethyl-1,6-heptadien-4-ol

Inchi: InChI=1S/C10H18O/c1-8(2)6-10(5,11)7-9(3)4/h11H,1,3,6-7H2,2,4-5H3
InchiKey: METKJWMTLIYYIQ-UHFFFAOYSA-N
Formula: C10H18O
SMILES: C=C(C)CC(C)(O)CC(=C)C
Mol. weight [g/mol]: 154.25
CAS: 79604-66-3

Physical Properties

Property code	Value	Unit	Source
gf	57.92	kJ/mol	Joback Method
hf	-179.43	kJ/mol	Joback Method
hfus	13.15	kJ/mol	Joback Method
hvap	52.06	kJ/mol	Joback Method
log10ws	-3.09		Crippen Method
logp	2.670		Crippen Method
mcvol	149.030	ml/mol	McGowan Method
pc	2568.89	kPa	Joback Method
tb	510.27	K	Joback Method
tc	688.76	K	Joback Method
tf	234.26	K	Joback Method
vc	0.568	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.07	J/mol×K	510.27	Joback Method
cpg	359.47	J/mol×K	540.02	Joback Method
cpg	372.15	J/mol×K	569.77	Joback Method
cpg	384.16	J/mol×K	599.52	Joback Method
cpg	395.52	J/mol×K	629.26	Joback Method
cpg	406.28	J/mol×K	659.01	Joback Method
cpg	416.46	J/mol×K	688.76	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C79604663&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume