3,5-Heptadienol, 2-ethylidene-6-methyl, isomer # 2

Inchi: InChI=1S/C10H16O/c1-4-10(8-11)7-5-6-9(2)3/h4-7,11H,8H2,1-3H3
InchiKey: FSTMFKMUZPMDAZ-UHFFFAOYSA-N
Formula: C10H16O
SMILES: CC=C(C=CC=C(C)C)CO
Mol. weight [g/mol]: 152.23

Physical Properties

Property code	Value	Unit	Source
gf	120.06	kJ/mol	Joback Method
hf	-69.88	kJ/mol	Joback Method
hfus	23.73	kJ/mol	Joback Method
hvap	54.57	kJ/mol	Joback Method
log10ws	-2.83		Crippen Method
logp	2.447		Crippen Method
mcvol	144.730	ml/mol	McGowan Method
pc	2712.67	kPa	Joback Method
rinpol	1245.00		NIST Webbook
rinpol	1245.00		NIST Webbook
tb	532.62	K	Joback Method
tc	717.13	K	Joback Method
tf	220.12	K	Joback Method
vc	0.556	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	326.14	J/mol×K	532.62	Joback Method
cpg	338.48	J/mol×K	563.37	Joback Method
cpg	350.12	J/mol×K	594.12	Joback Method
cpg	361.13	J/mol×K	624.87	Joback Method
cpg	371.55	J/mol×K	655.62	Joback Method
cpg	381.42	J/mol×K	686.38	Joback Method
cpg	390.80	J/mol×K	717.13	Joback Method

Sources

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=R643440&Units=SI
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
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

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