(E)-4, (Z)-7-decadienol-1

Inchi: InChI=1S/C10H18O/c1-2-3-4-5-6-7-8-9-10-11/h3-4,6-7,11H,2,5,8-10H2,1H3/b4-3-,7-6+
InchiKey: NKODDQZVUPANMP-WWVFNRLHSA-N
Formula: C10H18O
SMILES: CCC=CCC=CCCCO
Mol. weight [g/mol]: 154.25

Physical Properties

Property code	Value	Unit	Source
af	0.6156		Cheméo Relay (1.0)
gf	56.94	kJ/mol	Joback Method
hf	-257.45	kJ/mol	Cheméo Relay (1.0)
hfus	26.15	kJ/mol	Joback Method
hvap	80.05	kJ/mol	Cheméo Relay (1.0)
ie	8.88	eV	Cheméo Relay (1.0)
logp	2.671		Crippen Method
mcvol	149.030	ml/mol	McGowan Method
pc	2545.61	kPa	Joback Method
ripol	1862.00		NIST Webbook
tb	504.42	K	Cheméo Relay (1.0)
tc	686.76	K	Cheméo Relay (1.0)
tf	244.31	K	Cheméo Relay (1.0)
vc	0.520	m3/kmol	Cheméo Relay (1.0)

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	-2.92750e+01
Coeff. B	1.02782e+00
Coeff. C	-7.18200e-04
Coeff. D	2.12400e-07
Coeff. E	0.00000e+00

Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Information	Value
Property code	dvisc
Equation	Y = exp(A + B/T + C·ln(T) + D·T^E)
Y unit	Pa×s
Coeff. A	-1.49024e+01
Coeff. B	2.92411e+03
Coeff. C	0.00000e+00
Coeff. D	0.00000e+00
Coeff. E	0.00000e+00
Basis	predicted
Comment	Liquid phase. Joback/Reid (1987), valid from Tf to 0.7·Tc.
Temperature range (K), min.	253.12
Temperature range (K), max.	490.24

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R327232&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

Cheméo Relay (1.0):

Legend

af: Acentric Factor

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

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

ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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