Benzene, 1-(1-ethylpropyl)-3-(1-methylbutyl)-

Inchi: InChI=1S/C16H26/c1-5-9-13(4)15-10-8-11-16(12-15)14(6-2)7-3/h8,10-14H,5-7,9H2,1-4H
InchiKey: LJXJIICRXIAWQR-UHFFFAOYSA-N
Formula: C16H26
SMILES: CCCC(C)c1cccc(C(CC)CC)c1
Mol. weight [g/mol]: 218.38
CAS: 100945-39-9

Physical Properties

Property code	Value	Unit	Source
af	0.5221		Cheméo Relay (1.0)
hf	-172.59	kJ/mol	Cheméo Relay (1.0)
hfus	23.80	kJ/mol	Joback Method
hvap	70.37	kJ/mol	Cheméo Relay (1.0)
ie	8.22	eV	Cheméo Relay (1.0)
logp	5.494		Crippen Method
mcvol	212.540	ml/mol	McGowan Method
pc	1704.71	kPa	Joback Method
tb	544.40	K	Cheméo Relay (1.0)
tc	746.75	K	Cheméo Relay (1.0)
tf	230.53	K	Cheméo Relay (1.0)
vc	0.779	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	-3.46260e+01
Coeff. B	1.39728e+00
Coeff. C	-8.17160e-04
Coeff. D	1.78800e-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	-1.20977e+01
Coeff. B	1.87480e+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.	279.02
Temperature range (K), max.	555.87

Sources

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=C100945399&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

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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