

TRANS-(2-ETHYLCYCLOPENTYL)METHANOL

Inchi:	InChI=1S/C8H16O/c1-2-7-4-3-5-8(7)6-9/h7-9H,2-6H2,1H3/t7-,8+/m0/s1
InchiKey:	RMUDBYVEBKXDKI-UHFFFAOYSA-N
Formula:	C8H16O
SMILES:	CC[C@H]1CCCC[C@@H]1CO
Mol. weight [g/mol]:	128.21

Physical Properties

Property code	Value	Unit	Source
hf	-288.87	kJ/mol	Cheméo Relay (1.0)
hfus	15.57	kJ/mol	Joback Method
hvap	65.69	kJ/mol	Cheméo Relay (1.0)
ie	9.14	eV	Cheméo Relay (1.0)
logp	1.805		Crippen Method
mcvol	118.590	ml/mol	McGowan Method
rinpol	1058.00		NIST Webbook
rinpol	1058.00		NIST Webbook
tb	464.23	K	Cheméo Relay (1.0)
tf	273.32	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	275.57	J/mol×K	485.23	Joback Method
cpg	289.88	J/mol×K	515.82	Joback Method
cpg	303.53	J/mol×K	546.41	Joback Method
cpg	316.54	J/mol×K	577.01	Joback Method
cpg	328.93	J/mol×K	607.60	Joback Method
cpg	340.72	J/mol×K	638.19	Joback Method
cpg	351.92	J/mol×K	668.78	Joback Method
dvisc	0.0294410	Pa×s	247.40	Joback Method
dvisc	0.0075141	Pa×s	287.04	Joback Method
dvisc	0.0026713	Pa×s	326.68	Joback Method
dvisc	0.0011879	Pa×s	366.31	Joback Method
dvisc	0.0006188	Pa×s	405.95	Joback Method

dvisc	0.0003620	Pa×s	445.59	Joback Method
dvisc	0.0002312	Pa×s	485.23	Joback Method

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=C36258089&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

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

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