Benzene, (1-propylheptadecyl)-

Other names: Eicosane, 4-phenyl-
4-Phenyleicosane
Inchi: InChI=1S/C26H46/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-18-22-25(21-4-2)26-23-19-17-2(
InchiKey: RFNYELHDUBVQMR-UHFFFAOYSA-N
Formula: C26H46
SMILES: CCCCCCCCCCCCCCCCC(CCC)c1ccccc1
Mol. weight [g/mol]: 358.64
CAS: 2400-03-5

Physical Properties

Property code	Value	Unit	Source
gf	278.01	kJ/mol	Joback Method
hf	-348.72	kJ/mol	Joback Method
hfus	53.61	kJ/mol	Joback Method
hvap	75.36	kJ/mol	Joback Method
ie	9.00 ± 0.10	eV	NIST Webbook
log10ws	-9.77		Crippen Method
logp	9.442		Crippen Method
mcvol	353.440	ml/mol	McGowan Method
pc	877.91	kPa	Joback Method
tb	820.52	K	Joback Method
tc	1009.19	K	Joback Method
tf	394.20	K	Joback Method
vc	1.377	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1247.45	J/mol×K	1009.19	Joback Method
cpg	1132.76	J/mol×K	820.52	Joback Method
cpg	1154.64	J/mol×K	851.96	Joback Method
cpg	1175.33	J/mol×K	883.41	Joback Method
cpg	1194.89	J/mol×K	914.85	Joback Method
cpg	1213.40	J/mol×K	946.30	Joback Method

cpg	1230.90	J/mol×K	977.74	Joback Method
dvisc	0.0000410	Pa×s	820.52	Joback Method
dvisc	0.0017071	Pa×s	394.20	Joback Method
dvisc	0.0005703	Pa×s	465.25	Joback Method
dvisc	0.0002548	Pa×s	536.31	Joback Method
dvisc	0.0001374	Pa×s	607.36	Joback Method
dvisc	0.0000844	Pa×s	678.41	Joback Method
dvisc	0.0000568	Pa×s	749.47	Joback Method
hvapt	88.20	kJ/mol	507.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2400035&Units=SI
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

Legend

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
hvapt: Enthalpy of vaporization at a given temperature
ie: Ionization energy
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

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