4-C14H26

Other names: 4-C14H26
Inchi: InChI=1S/C14H26/c1-3-5-7-9-11-13-14-12-10-8-6-4-2/h3-7,9,11-14H2,1-2H3
InchiKey: QWZXVDGVISCHQH-UHFFFAOYSA-N
Formula: C14H26
SMILES: CCCC#CCCCCCCCCC
Mol. weight [g/mol]: 194.36

Physical Properties

Property code	Value	Unit	Source
af	0.5427		Cheméo Relay (1.0)
gf	269.80	kJ/mol	Joback Method
hf	-60.09	kJ/mol	Cheméo Relay (1.0)
hfus	35.14	kJ/mol	Joback Method
hvap	65.93	kJ/mol	Cheméo Relay (1.0)
ie	9.11 ± 0.03	eV	NIST Webbook
log10ws	-6.19		Cheméo Relay (1.0)
logp	4.931		Crippen Method
mcvol	199.520	ml/mol	McGowan Method
pc	1733.22	kPa	Joback Method
rinpol	1406.00		NIST Webbook
rinpol	1407.00		NIST Webbook
rinpol	1427.00		NIST Webbook
rinpol	1407.00		NIST Webbook
ripol	1586.00		NIST Webbook
ripol	1586.00		NIST Webbook
ripol	1557.80		NIST Webbook
ripol	1576.00		NIST Webbook
ripol	1576.30		NIST Webbook
ripol	1584.00		NIST Webbook
ripol	1585.00		NIST Webbook
ripol	1576.00		NIST Webbook
ripol	1557.80		NIST Webbook
ripol	1586.00		NIST Webbook
ripol	1553.60		NIST Webbook
tb	503.90	K	Cheméo Relay (1.0)
tc	700.22	K	Cheméo Relay (1.0)
tf	251.29	K	Cheméo Relay (1.0)

vc	0.772	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	473.12	J/mol×K	528.72	Joback Method
cpg	490.92	J/mol×K	558.32	Joback Method
cpg	507.98	J/mol×K	587.93	Joback Method
cpg	524.33	J/mol×K	617.53	Joback Method
cpg	539.98	J/mol×K	647.14	Joback Method
cpg	554.96	J/mol×K	676.74	Joback Method
cpg	569.28	J/mol×K	706.35	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=C60212331&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
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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume