

pentacontane

Inchi: InChI=1S/C50H102/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-31-33-35-37-39-41-43-45
InchiKey: PFLUOWJPZLHUEA-UHFFFAOYSA-N
Formula: C50H102
SMILES: CC
Mol. weight [g/mol]: 703.34
CAS: 6596-40-3

Physical Properties

Property code	Value	Unit	Source
gf	370.12	kJ/mol	Joback Method
hf	-1075.33	kJ/mol	Joback Method
hfus	125.26	kJ/mol	Joback Method
hvap	252.50 ± 0.20	kJ/mol	NIST Webbook
log10ws	-20.75		Crippen Method
logp	19.751		Crippen Method
mvol	715.360	ml/mol	McGowan Method
pc	276.12	kPa	Joback Method
tb	1343.40	K	Joback Method
tc	2196.22	K	Joback Method
tf	365.30 ± 2.00	K	NIST Webbook
tf	365.30 ± 1.50	K	NIST Webbook
tf	366.20 ± 3.00	K	NIST Webbook
vc	2.836	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	3577.43	J/mol×K	2196.22	Joback Method
cpg	2893.25	J/mol×K	1343.40	Joback Method
cpg	2983.29	J/mol×K	1485.54	Joback Method
cpg	3069.52	J/mol×K	1627.67	Joback Method
cpg	3161.98	J/mol×K	1769.81	Joback Method
cpg	3270.75	J/mol×K	1911.95	Joback Method
cpg	3405.88	J/mol×K	2054.08	Joback Method

dvisc	0.0000009	Paxs	1343.40	Joback Method
dvisc	0.0000475	Paxs	653.26	Joback Method
dvisc	0.0000151	Paxs	768.28	Joback Method
dvisc	0.0000064	Paxs	883.31	Joback Method
dvisc	0.0000033	Paxs	998.33	Joback Method
dvisc	0.0000020	Paxs	1113.35	Joback Method
dvisc	0.0000013	Paxs	1228.38	Joback Method
hfust	185.00	kJ/mol	366.90	NIST Webbook
hfust	185.00	kJ/mol	366.90	NIST Webbook
hvapt	149.00	kJ/mol	727.50	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6596403&Units=SI

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
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mvol:	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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