1,8,15-Hexadecatriyne

Inchi: InChI=1S/C16H22/c1-3-5-7-9-11-13-15-16-14-12-10-8-6-4-2/h1-2H,5-14H2
InchiKey: FQMIMRQHPBBFQF-UHFFFAOYSA-N
Formula: C16H22
SMILES: C#CCCCCCC#CCCCCCC#C
Mol. weight [g/mol]: 214.35
CAS: 4580-43-2

Physical Properties

Property code	Value	Unit	Source
gf	732.78	kJ/mol	Joback Method
hf	482.53	kJ/mol	Joback Method
hfus	46.27	kJ/mol	Joback Method
hvap	53.08	kJ/mol	Joback Method
log10ws	-5.90		Crippen Method
logp	4.157		Crippen Method
mcvol	210.500	ml/mol	McGowan Method
pc	1893.65	kPa	Joback Method
tb	554.72	K	Joback Method
tc	751.30	K	Joback Method
tf	470.12	K	Joback Method
vc	0.818	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	495.09	J/mol×K	554.72	Joback Method
cpg	512.28	J/mol×K	587.48	Joback Method
cpg	528.60	J/mol×K	620.25	Joback Method
cpg	544.10	J/mol×K	653.01	Joback Method
cpg	558.82	J/mol×K	685.77	Joback Method
cpg	572.79	J/mol×K	718.53	Joback Method
cpg	586.07	J/mol×K	751.30	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	386.00 ± 1.00	K	0.10	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4580432&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
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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume