

1,8,15,22-Tricosatetrayne

Inchi:	InChI=1S/C23H32/c1-3-5-7-9-11-13-15-17-19-21-23-22-20-18-16-14-12-10-8-6-4-2/h1-21
InchiKey:	GXFDRUIKMBUYRC-UHFFFAOYSA-N
Formula:	C23H32
SMILES:	C#CCCCCCC#CCCCCCC#CCCCCCC#C
Mol. weight [g/mol]:	308.50
CAS:	4641-78-5

Physical Properties

Property code	Value	Unit	Source
gf	994.52	kJ/mol	Joback Method
hf	610.35	kJ/mol	Joback Method
hfus	67.52	kJ/mol	Joback Method
hvap	70.81	kJ/mol	Joback Method
log10ws	-8.63		Crippen Method
logp	6.111		Crippen Method
mcvol	300.530	ml/mol	McGowan Method
pc	1266.45	kPa	Joback Method
tb	723.88	K	Joback Method
tc	923.52	K	Joback Method
tf	655.11	K	Joback Method
vc	1.171	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	831.51	J/mol×K	723.88	Joback Method
cpg	851.20	J/mol×K	757.15	Joback Method
cpg	869.89	J/mol×K	790.43	Joback Method
cpg	887.65	J/mol×K	823.70	Joback Method
cpg	904.51	J/mol×K	856.97	Joback Method
cpg	920.56	J/mol×K	890.25	Joback Method
cpg	935.83	J/mol×K	923.52	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	443.00	K	0.01	NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4641785&Units=SI

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

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