

8,12,20-trimethyltetracontane

Inchi: InChI=1S/C43H88/c1-6-8-10-12-13-14-15-16-17-18-19-20-21-22-23-24-27-31-35-41(3)36
InchiKey: VUFKLWVJAXLPHF-UHFFFAOYSA-N
Formula: C43H88
SMILES: CCCCCCCCCCCCCCCCCCCCCC(C)CCCCCCCC(C)CCCC(C)CCCCCCC
Mol. weight [g/mol]: 605.16

Physical Properties

Property code	Value	Unit	Source
gf	303.86	kJ/mol	Joback Method
hf	-946.69	kJ/mol	Joback Method
hfus	96.56	kJ/mol	Joback Method
hvap	110.15	kJ/mol	Joback Method
log10ws	-17.10		Crippen Method
logp	16.588		Crippen Method
mcvol	616.730	ml/mol	McGowan Method
pc	353.06	kPa	Joback Method
rinpol	4084.00		NIST Webbook
rinpol	4084.00		NIST Webbook
tb	1181.92	K	Joback Method
tc	1624.44	K	Joback Method
tf	529.37	K	Joback Method
vc	2.425	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2388.44	J/mol×K	1181.92	Joback Method
cpg	2437.38	J/mol×K	1255.67	Joback Method
cpg	2481.48	J/mol×K	1329.43	Joback Method
cpg	2521.94	J/mol×K	1403.18	Joback Method
cpg	2559.95	J/mol×K	1476.94	Joback Method
cpg	2596.73	J/mol×K	1550.69	Joback Method
cpg	2633.46	J/mol×K	1624.44	Joback Method
dvisc	0.0002373	Pa×s	529.37	Joback Method

dvisc	0.0000562	Pa×s	638.13	Joback Method
dvisc	0.0000203	Pa×s	746.89	Joback Method
dvisc	0.0000095	Pa×s	855.64	Joback Method
dvisc	0.0000052	Pa×s	964.40	Joback Method
dvisc	0.0000033	Pa×s	1073.16	Joback Method
dvisc	0.0000022	Pa×s	1181.92	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R280658&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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