Dodecane, 5-butyl-6-ethyl

Inchi: InChI=1S/C18H38/c1-5-9-12-13-16-17(8-4)18(14-10-6-2)15-11-7-3/h17-18H,5-16H2,1-4H
InchiKey: JXACHSBKZJSUFZ-UHFFFAOYSA-N
Formula: C18H38
SMILES: CCCCCCC(CC)C(CCCC)CCCC
Mol. weight [g/mol]: 254.49

Physical Properties

Property code	Value	Unit	Source
gf	95.80	kJ/mol	Joback Method
hf	-425.41	kJ/mol	Joback Method
hfus	35.33	kJ/mol	Joback Method
hvap	54.89	kJ/mol	Joback Method
log10ws	-6.87		Crippen Method
logp	6.980		Crippen Method
mcvol	264.480	ml/mol	McGowan Method
pc	1164.84	kPa	Joback Method
rinpol	1582.00		NIST Webbook
tb	610.36	K	Joback Method
tc	773.50	K	Joback Method
tf	262.62	K	Joback Method
vc	1.032	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	724.07	J/mol×K	610.36	Joback Method
cpg	744.77	J/mol×K	637.55	Joback Method
cpg	764.63	J/mol×K	664.74	Joback Method
cpg	783.65	J/mol×K	691.93	Joback Method
cpg	801.88	J/mol×K	719.12	Joback Method
cpg	819.32	J/mol×K	746.31	Joback Method
cpg	836.01	J/mol×K	773.50	Joback Method
dvisc	0.0097660	Pa×s	262.62	Joback Method
dvisc	0.0023312	Pa×s	320.58	Joback Method

dvisc	0.0008629	Pa×s	378.53	Joback Method
dvisc	0.0004158	Pa×s	436.49	Joback Method
dvisc	0.0002378	Pa×s	494.45	Joback Method
dvisc	0.0001529	Pa×s	552.40	Joback Method
dvisc	0.0001069	Pa×s	610.36	Joback Method

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=R8978&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
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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