

Octadecane, 3-ethyl-5-(2-ethylbutyl)-

Other names:	3-Ethyl-5-(2'-ethylbutyl)octadecane 3-Ethyl-5-(2-ethylbutyl)octadecane
Inchi:	InChI=1S/C26H54/c1-6-11-12-13-14-15-16-17-18-19-20-21-26(22-24(7-2)8-3)23-25(9-4)
InchiKey:	MFLJAIATZVGFPM-UHFFFAOYSA-N
Formula:	C26H54
SMILES:	CCCCCCCCCCCC(CC(CC)CC)CC(CC)CC
Mol. weight [g/mol]:	366.71
CAS:	55282-12-7

Physical Properties

Property code	Value	Unit	Source
gf	160.72	kJ/mol	Joback Method
hf	-595.81	kJ/mol	Joback Method
hfus	52.53	kJ/mol	Joback Method
hvap	72.31	kJ/mol	Joback Method
log10ws	-9.98		Crippen Method
logp	9.956		Crippen Method
mvol	377.200	ml/mol	McGowan Method
pc	734.42	kPa	Joback Method
tb	792.96	K	Joback Method
tc	971.41	K	Joback Method
tf	337.78	K	Joback Method
vc	1.474	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1345.27	J/molxK	971.41	Joback Method
cpg	1326.61	J/molxK	941.67	Joback Method
cpg	1306.95	J/molxK	911.93	Joback Method
cpg	1286.26	J/molxK	882.19	Joback Method
cpg	1264.47	J/molxK	852.44	Joback Method
cpg	1241.56	J/molxK	822.70	Joback Method
cpg	1217.46	J/molxK	792.96	Joback Method

dvisc	0.0044687	Paxs	337.78	Joback Method
dvisc	0.0000339	Paxs	792.96	Joback Method
dvisc	0.0000498	Paxs	717.10	Joback Method
dvisc	0.0000799	Paxs	641.23	Joback Method
dvisc	0.0001458	Paxs	565.37	Joback Method
dvisc	0.0003203	Paxs	489.51	Joback Method
dvisc	0.0009396	Paxs	413.64	Joback Method
hvapt	88.40	kJ/mol	485.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.68219e+01
Coeff. B	-6.55756e+03
Coeff. C	-1.31677e+02
Temperature range (K), min.	528.28
Temperature range (K), max.	701.38

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55282127&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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