

Triacontane, 1-bromo-

Inchi:	InChI=1S/C30H61Br/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24
InchiKey:	SFVIZKWTUKBDIY-UHFFFAOYSA-N
Formula:	C30H61Br
SMILES:	CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCBr
Mol. weight [g/mol]:	501.71
CAS:	4209-22-7

Physical Properties

Property code	Value	Unit	Source
gf	216.04	kJ/mol	Joback Method
hf	-636.20	kJ/mol	Joback Method
hfus	78.74	kJ/mol	Joback Method
hvap	88.81	kJ/mol	Joback Method
log10ws	-12.81		Crippen Method
logp	12.324		Crippen Method
mcvol	451.060	ml/mol	McGowan Method
pc	616.04	kPa	Joback Method
tb	951.96	K	Joback Method
tc	1177.94	K	Joback Method
tf	339.60 ± 0.50	K	NIST Webbook
tf	339.60 ± 0.60	K	NIST Webbook
vc	1.778	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1542.53	J/molxK	951.96	Joback Method
cpg	1569.09	J/molxK	989.62	Joback Method
cpg	1594.09	J/molxK	1027.29	Joback Method
cpg	1617.64	J/molxK	1064.95	Joback Method
cpg	1639.86	J/molxK	1102.61	Joback Method
cpg	1660.89	J/molxK	1140.28	Joback Method
cpg	1680.84	J/molxK	1177.94	Joback Method
dvisc	0.0005537	Paxs	487.66	Joback Method

dvisc	0.0002119	Paxs	565.04	Joback Method
dvisc	0.0001022	Paxs	642.43	Joback Method
dvisc	0.0000577	Paxs	719.81	Joback Method
dvisc	0.0000364	Paxs	797.19	Joback Method
dvisc	0.0000249	Paxs	874.58	Joback Method
dvisc	0.0000181	Paxs	951.96	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4209227&Units=SI

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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