

Pentacosane, 1-bromo-

Inchi:	InChI=1S/C25H51Br/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:	DDEOKNGWYRTQDY-UHFFFAOYSA-N
Formula:	C25H51Br
SMILES:	CCCCCCCCCCCCCCCCCCCCCCCCCCCCBr
Mol. weight [g/mol]:	431.58
CAS:	62108-45-6

Physical Properties

Property code	Value	Unit	Source
gf	173.94	kJ/mol	Joback Method
hf	-533.00	kJ/mol	Joback Method
hfus	65.79	kJ/mol	Joback Method
hvap	77.68	kJ/mol	Joback Method
log10ws	-10.72		Crippen Method
logp	10.373		Crippen Method
mcvol	380.610	ml/mol	McGowan Method
pc	793.94	kPa	Joback Method
tb	837.56	K	Joback Method
tc	1025.41	K	Joback Method
tf	431.31	K	Joback Method
vc	1.498	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1213.56	J/molxK	837.56	Joback Method
cpg	1314.84	J/molxK	994.10	Joback Method
cpg	1296.59	J/molxK	962.79	Joback Method
cpg	1277.40	J/molxK	931.49	Joback Method
cpg	1257.20	J/molxK	900.18	Joback Method
cpg	1235.95	J/molxK	868.87	Joback Method
cpg	1332.20	J/molxK	1025.41	Joback Method
dvisc	0.0000392	Paxs	837.56	Joback Method
dvisc	0.0000535	Paxs	769.85	Joback Method

dvisc	0.0000773	Paxs	702.14	Joback Method
dvisc	0.0001211	Paxs	634.44	Joback Method
dvisc	0.0002110	Paxs	566.73	Joback Method
dvisc	0.0004275	Paxs	499.02	Joback Method
dvisc	0.0010812	Paxs	431.31	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C62108456&Units=SI
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
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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