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: CCCCCCCCCCCCCCCCCCCCCCCCCBr
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/mol×K	837.56	Joback Method
cpg	1235.95	J/mol×K	868.87	Joback Method
cpg	1257.20	J/mol×K	900.18	Joback Method
cpg	1277.40	J/mol×K	931.49	Joback Method
cpg	1296.59	J/mol×K	962.79	Joback Method
cpg	1314.84	J/mol×K	994.10	Joback Method
cpg	1332.20	J/mol×K	1025.41	Joback Method
dvisc	0.0010812	Pa×s	431.31	Joback Method
dvisc	0.0004275	Pa×s	499.02	Joback Method

dvisc	0.0002110	Pa×s	566.73	Joback Method
dvisc	0.0001211	Pa×s	634.44	Joback Method
dvisc	0.0000773	Pa×s	702.14	Joback Method
dvisc	0.0000535	Pa×s	769.85	Joback Method
dvisc	0.0000392	Pa×s	837.56	Joback Method

Sources

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=C62108456&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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