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: CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCBr
Mol. weight [g/mol]: 501.72

Physical Properties

Property code	Value	Unit	Source
af	1.3211		Cheméo Relay (1.0)
gf	216.04	kJ/mol	Joback Method
hf	-666.18	kJ/mol	Cheméo Relay (1.0)
hfus	78.74	kJ/mol	Joback Method
hvap	164.73	kJ/mol	Cheméo Relay (1.0)
ie	10.40	eV	Cheméo Relay (1.0)
log10ws	-11.53		Cheméo Relay (1.0)
logp	12.324		Crippen Method
mcvol	451.060	ml/mol	McGowan Method
pc	616.04	kPa	Joback Method
tb	670.87	K	Cheméo Relay (1.0)
tc	843.70	K	Cheméo Relay (1.0)
tf	339.60 ± 0.50	K	NIST Webbook
tf	339.60 ± 0.60	K	NIST Webbook
vc	1.785	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

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

dvisc	0.0000577	Pa×s	719.81	Joback Method
dvisc	0.0000181	Pa×s	951.96	Joback Method
dvisc	0.0000249	Pa×s	874.58	Joback Method
dvisc	0.0000364	Pa×s	797.19	Joback Method
dvisc	0.0005537	Pa×s	487.66	Joback Method
dvisc	0.0001022	Pa×s	642.43	Joback Method
dvisc	0.0002119	Pa×s	565.04	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4209227&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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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