Tetrabromo-o-xylene

Inchi: InChI=1S/C8H6Br4/c1-3-4(2)6(10)8(12)7(11)5(3)9/h1-2H3
InchiKey: WVJRAJZMOVQFEC-UHFFFAOYSA-N
Formula: C8H6Br4
SMILES: Cc1c(C)c(Br)c(Br)c(Br)c1Br
Mol. weight [g/mol]: 421.75
CAS: 36059-21-9

Physical Properties

Property code	Value	Unit	Source
hfus	29.71	kJ/mol	Joback Method
ie	8.34	eV	Cheméo Relay (1.0)
logp	5.353		Crippen Method
mcvol	169.820	ml/mol	McGowan Method
tb	620.41	K	Cheméo Relay (1.0)
tf	535.15	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	6.59700e+01
Coeff. B	5.40240e-01
Coeff. C	-3.93000e-04
Coeff. D	1.21400e-07
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Information	Value

Property code	dvisc
Equation	Y = exp(A + B/T + C·ln(T) + D·T^E)
Y unit	Pa×s
Coeff. A	-1.12756e+01
Coeff. B	1.97996e+03
Coeff. C	0.00000e+00
Coeff. D	0.00000e+00
Coeff. E	0.00000e+00
Basis	predicted
Comment	Liquid phase. Joback/Reid (1987), valid from Tf to 0.7·Tc.
Temperature range (K), min.	535.15
Temperature range (K), max.	681.92

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Jean-Claude Bradley Open Melting Point Dataset (2014, CC0): https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Datset/1031637

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hfus: Enthalpy of fusion at standard conditions
ie: Ionization energy
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point

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