2,4-Bis(trifluoromethyl)benzyl bromide

Inchi: InChI=1S/C9H5BrF6/c10-4-5-1-2-6(8(11,12)13)3-7(5)9(14,15)16/h1-3H,4H2
InchiKey: SWFFFUJOWAJJCH-UHFFFAOYSA-N
Formula: C9H5BrF6
SMILES: FC(F)(F)c1ccc(CBr)c(C(F)(F)F)c1
Mol. weight [g/mol]: 307.03
CAS: 140690-56-8

Physical Properties

Property code	Value	Unit	Source
gf	-1030.81	kJ/mol	Joback Method
hf	-1183.33	kJ/mol	Joback Method
hfus	21.27	kJ/mol	Joback Method
hvap	38.17	kJ/mol	Joback Method
log10ws	-4.99		Crippen Method
logp	4.619		Crippen Method
mcvol	142.030	ml/mol	McGowan Method
pc	2646.11	kPa	Joback Method
tb	497.28	K	Joback Method
tc	685.79	K	Joback Method
tf	310.83	K	Joback Method
vc	0.580	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	311.27	J/mol×K	497.28	Joback Method
cpg	322.14	J/mol×K	528.70	Joback Method
cpg	332.17	J/mol×K	560.12	Joback Method
cpg	341.41	J/mol×K	591.54	Joback Method
cpg	349.90	J/mol×K	622.95	Joback Method
cpg	357.72	J/mol×K	654.37	Joback Method
cpg	364.89	J/mol×K	685.79	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C140690568&Units=SI

Legend

cpg:	Ideal gas heat capacity
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

Latest version available from:
https://www.chemeo.com/cid/19-181-0/2-4-Bis-trifluoromethyl-benzyl-bromide.pdf
Generated by Cheméo on 2024-04-28 19:24:39.650376106 +0000 UTC m=+16621528.570953428.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.