7-Bromo-1-heptanol, chlorodifluoroacetate

Inchi: InChI=1S/C9H14BrClF2O2/c10-6-4-2-1-3-5-7-15-8(14)9(11,12)13/h1-7H2
InchiKey: BHEGXDUPLKVMPM-UHFFFAOYSA-N
Formula: C9H14BrClF2O2
SMILES: O=C(OCCCCCCCBr)C(F)(F)Cl
Mol. weight [g/mol]: 307.56

Physical Properties

Property code	Value	Unit	Source
gf	-593.41	kJ/mol	Joback Method
hf	-864.27	kJ/mol	Joback Method
hfus	30.08	kJ/mol	Joback Method
hvap	52.67	kJ/mol	Joback Method
log10ws	-3.85		Crippen Method
logp	3.707		Crippen Method
mcvol	178.390	ml/mol	McGowan Method
pc	2322.54	kPa	Joback Method
rinpol	1494.00		NIST Webbook
rinpol	1494.00		NIST Webbook
tb	580.51	K	Joback Method
tc	765.94	K	Joback Method
tf	356.67	K	Joback Method
vc	0.700	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	412.62	J/mol×K	580.51	Joback Method
cpg	424.26	J/mol×K	611.42	Joback Method
cpg	435.26	J/mol×K	642.32	Joback Method
cpg	445.62	J/mol×K	673.23	Joback Method
cpg	455.39	J/mol×K	704.13	Joback Method
cpg	464.58	J/mol×K	735.04	Joback Method
cpg	473.24	J/mol×K	765.94	Joback Method

Sources

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=U376263&Units=SI
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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume