5-Bromovaleric acid, dodec-9-ynyl ester

Inchi: InChI=1S/C17H29BrO2/c1-2-3-4-5-6-7-8-9-10-13-16-20-17(19)14-11-12-15-18/h2,5-16H
InchiKey: QRNDLYLSRJZIBH-UHFFFAOYSA-N
Formula: C17H29BrO2
SMILES: CCC#CCCCCCCCCOC(=O)CCCCBr
Mol. weight [g/mol]: 345.31

Physical Properties

Property code	Value	Unit	Source
gf	75.46	kJ/mol	Joback Method
hf	-340.38	kJ/mol	Joback Method
hfus	50.98	kJ/mol	Joback Method
hvap	71.18	kJ/mol	Joback Method
log10ws	-6.03		Crippen Method
logp	5.239		Crippen Method
mcvol	266.730	ml/mol	McGowan Method
pc	1508.15	kPa	Joback Method
rinpol	2262.00		NIST Webbook
rinpol	2262.00		NIST Webbook
tb	739.81	K	Joback Method
tc	931.60	K	Joback Method
tf	519.41	K	Joback Method
vc	1.036	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	739.66	J/mol×K	739.81	Joback Method
cpg	756.34	J/mol×K	771.78	Joback Method
cpg	772.16	J/mol×K	803.74	Joback Method
cpg	787.14	J/mol×K	835.71	Joback Method
cpg	801.30	J/mol×K	867.67	Joback Method
cpg	814.67	J/mol×K	899.64	Joback Method
cpg	827.28	J/mol×K	931.60	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299985&Units=SI
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

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

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