5-Bromovaleric acid, tridec-2-ynyl ester

Inchi: InChI=1S/C18H31BrO2/c1-2-3-4-5-6-7-8-9-10-11-14-17-21-18(20)15-12-13-16-19/h2-10,
InchiKey: JUXZXAPWMXWRKX-UHFFFAOYSA-N
Formula: C18H31BrO2
SMILES: CCCCCCCCCCC#CCOC(=O)CCCCBr
Mol. weight [g/mol]: 359.34

Physical Properties

Property code	Value	Unit	Source
gf	83.88	kJ/mol	Joback Method
hf	-361.02	kJ/mol	Joback Method
hfus	53.57	kJ/mol	Joback Method
hvap	73.41	kJ/mol	Joback Method
log10ws	-6.45		Crippen Method
logp	5.629		Crippen Method
mcvol	280.820	ml/mol	McGowan Method
pc	1401.69	kPa	Joback Method
rinpol	2367.10		NIST Webbook
rinpol	2367.10		NIST Webbook
tb	762.69	K	Joback Method
tc	954.00	K	Joback Method
tf	530.68	K	Joback Method
vc	1.091	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	796.87	J/mol×K	762.69	Joback Method
cpg	813.91	J/mol×K	794.58	Joback Method
cpg	830.06	J/mol×K	826.46	Joback Method
cpg	845.33	J/mol×K	858.35	Joback Method
cpg	859.76	J/mol×K	890.23	Joback Method
cpg	873.38	J/mol×K	922.12	Joback Method
cpg	886.22	J/mol×K	954.00	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=U292570&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
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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