6-Bromohexanoic acid, tridec-2-ynyl ester

Inchi: InChI=1S/C19H33BrO2/c1-2-3-4-5-6-7-8-9-10-11-15-18-22-19(21)16-13-12-14-17-20/h2-
InchiKey: QZODGTJJDJNAKI-UHFFFAOYSA-N
Formula: C19H33BrO2
SMILES: CCCCCCCCCCC#CCOC(=O)CCCCCBr
Mol. weight [g/mol]: 373.37

Physical Properties

Property code	Value	Unit	Source
gf	92.30	kJ/mol	Joback Method
hf	-381.66	kJ/mol	Joback Method
hfus	56.16	kJ/mol	Joback Method
hvap	75.63	kJ/mol	Joback Method
log10ws	-6.86		Crippen Method
logp	6.019		Crippen Method
mcvol	294.910	ml/mol	McGowan Method
pc	1306.12	kPa	Joback Method
rinpol	2410.00		NIST Webbook
rinpol	2410.00		NIST Webbook
tb	785.57	K	Joback Method
tc	976.98	K	Joback Method
tf	541.95	K	Joback Method
vc	1.147	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	855.11	J/mol×K	785.57	Joback Method
cpg	872.49	J/mol×K	817.47	Joback Method
cpg	888.94	J/mol×K	849.37	Joback Method
cpg	904.50	J/mol×K	881.27	Joback Method
cpg	919.18	J/mol×K	913.17	Joback Method
cpg	933.04	J/mol×K	945.08	Joback Method
cpg	946.09	J/mol×K	976.98	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=U299295&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