

5-Bromovaleric acid, 2-tridecyl ester

Inchi:	InChI=1S/C18H35BrO2/c1-3-4-5-6-7-8-9-10-11-14-17(2)21-18(20)15-12-13-16-19/h17H,
InchiKey:	ULANFQWUXUFDTM-UHFFFAOYSA-N
Formula:	C18H35BrO2
SMILES:	CCCCCCCCCCCC(C)OC(=O)CCCCBr
Mol. weight [g/mol]:	363.37

Physical Properties

Property code	Value	Unit	Source
gf	-121.36	kJ/mol	Joback Method
hf	-638.60	kJ/mol	Joback Method
hfus	46.92	kJ/mol	Joback Method
hvap	70.86	kJ/mol	Joback Method
log10ws	-6.76		Crippen Method
logp	6.404		Crippen Method
mcvol	289.420	ml/mol	McGowan Method
pc	1254.81	kPa	Joback Method
rinpol	2215.00		NIST Webbook
tb	753.25	K	Joback Method
tc	934.86	K	Joback Method
tf	409.58	K	Joback Method
vc	1.123	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	844.38	J/molxK	753.25	Joback Method
cpg	862.22	J/molxK	783.52	Joback Method
cpg	879.15	J/molxK	813.79	Joback Method
cpg	895.20	J/molxK	844.05	Joback Method
cpg	910.40	J/molxK	874.32	Joback Method
cpg	924.79	J/molxK	904.59	Joback Method
cpg	938.38	J/molxK	934.86	Joback Method
dvisc	0.0014522	Paxs	409.58	Joback Method
dvisc	0.0006475	Paxs	466.86	Joback Method

dvisc	0.0003445	Paxs	524.14	Joback Method
dvisc	0.0002075	Paxs	581.41	Joback Method
dvisc	0.0001369	Paxs	638.69	Joback Method
dvisc	0.0000967	Paxs	695.97	Joback Method
dvisc	0.0000721	Paxs	753.25	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=U299924&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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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