Octadecanoic acid, 9,10-dibromo-, methyl ester

Other names: Methyl 9,10-dibromostearate
9,10-Dibromostearic acid methyl ester
Methyl 9,10-dibromooctadecanoate

Inchi: InChI=1S/C19H36Br2O2/c1-3-4-5-6-8-11-14-17(20)18(21)15-12-9-7-10-13-16-19(22)23-2

InchiKey: QNMTXFWVHQDSNR-UHFFFAOYSA-N

Formula: C19H36Br2O2

SMILES: CCCCCCCCC(Br)C(Br)CCCCCCCC(=O)OC

Mol. weight [g/mol]: 456.30

CAS: 25456-04-6

Physical Properties

Property code	Value	Unit	Source
gf	-101.06	kJ/mol	Joback Method
hf	-638.19	kJ/mol	Joback Method
hfus	51.28	kJ/mol	Joback Method
hvap	79.14	kJ/mol	Joback Method
log10ws	-7.73		Crippen Method
logp	7.168		Crippen Method
mcvol	321.010	ml/mol	McGowan Method
pc	1238.09	kPa	Joback Method
tb	841.85	K	Joback Method
tc	1037.90	K	Joback Method
tf	465.65	K	Joback Method
vc	1.236	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	952.48	J/mol×K	841.85	Joback Method
cpg	969.52	J/mol×K	874.53	Joback Method
cpg	985.59	J/mol×K	907.20	Joback Method
cpg	1000.72	J/mol×K	939.88	Joback Method
cpg	1014.97	J/mol×K	972.55	Joback Method
cpg	1028.39	J/mol×K	1005.23	Joback Method

cpg	1041.01	J/mol×K	1037.90	Joback Method
dvisc	0.0008625	Pa×s	465.65	Joback Method
dvisc	0.0003901	Pa×s	528.35	Joback Method
dvisc	0.0002088	Pa×s	591.05	Joback Method
dvisc	0.0001260	Pa×s	653.75	Joback Method
dvisc	0.0000831	Pa×s	716.45	Joback Method
dvisc	0.0000586	Pa×s	779.15	Joback Method
dvisc	0.0000435	Pa×s	841.85	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=C25456046&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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