5-bromovaleric acid, hexadecyl ester

Inchi: InChI=1S/C21H41BrO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-17-20-24-21(23)18-15-16-19-
InchiKey: NXIGXKBOTAEOKV-UHFFFAOYSA-N
Formula: C21H41BrO2
SMILES: CCCCCCCCCCCCCCCCOC(=O)CCCCBr
Mol. weight [g/mol]: 405.46

Physical Properties

Property code	Value	Unit	Source
af	1.0998		Cheméo Relay (1.0)
hf	-787.84	kJ/mol	Cheméo Relay (1.0)
hfus	58.22	kJ/mol	Joback Method
hvap	111.07	kJ/mol	Cheméo Relay (1.0)
ie	9.80	eV	Cheméo Relay (1.0)
log10ws	-7.53		Cheméo Relay (1.0)
logp	7.576		Crippen Method
mcvol	331.690	ml/mol	McGowan Method
pc	1027.94	kPa	Joback Method
rinpol	2640.00		NIST Webbook
rinpol	2640.00		NIST Webbook
tb	634.16	K	Cheméo Relay (1.0)
tc	811.38	K	Cheméo Relay (1.0)
tf	310.08	K	Cheméo Relay (1.0)
vc	1.268	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1024.15	J/mol×K	822.33	Joback Method
cpg	1123.30	J/mol×K	1008.86	Joback Method
cpg	1109.06	J/mol×K	977.77	Joback Method
cpg	1093.96	J/mol×K	946.68	Joback Method
cpg	1077.96	J/mol×K	915.59	Joback Method
cpg	1061.01	J/mol×K	884.51	Joback Method
cpg	1043.09	J/mol×K	853.42	Joback Method

dvisc	0.0001394	Pa×s	640.36	Joback Method
dvisc	0.0000504	Pa×s	822.33	Joback Method
dvisc	0.0000671	Pa×s	761.67	Joback Method
dvisc	0.0000937	Pa×s	701.02	Joback Method
dvisc	0.0008628	Pa×s	458.39	Joback Method
dvisc	0.0002253	Pa×s	579.70	Joback Method
dvisc	0.0004077	Pa×s	519.05	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U292293&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
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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