

3-Methoxybutyl caprate

Inchi:	InChI=1S/C15H30O3/c1-4-5-6-7-8-9-10-11-15(16)18-13-12-14(2)17-3/h14H,4-13H2,1-3H
InchiKey:	DCVHHJWODOXCLN-UHFFFAOYSA-N
Formula:	C15H30O3
SMILES:	CCCCCCCCC(=O)OCCC(C)OC
Mol. weight [g/mol]:	258.40

Physical Properties

Property code	Value	Unit	Source
gf	-265.94	kJ/mol	Joback Method
hf	-735.23	kJ/mol	Joback Method
hfus	35.06	kJ/mol	Joback Method
hvap	60.16	kJ/mol	Joback Method
log10ws	-4.16		Crippen Method
logp	4.095		Crippen Method
mcvol	235.520	ml/mol	McGowan Method
pc	1455.68	kPa	Joback Method
rinpol	1725.00		NIST Webbook
tb	640.87	K	Joback Method
tc	811.05	K	Joback Method
tf	338.20	K	Joback Method
vc	0.911	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	651.33	J/molxK	640.87	Joback Method
cpg	731.33	J/molxK	782.69	Joback Method
cpg	716.78	J/molxK	754.32	Joback Method
cpg	701.51	J/molxK	725.96	Joback Method
cpg	685.51	J/molxK	697.60	Joback Method
cpg	668.79	J/molxK	669.23	Joback Method
cpg	745.18	J/molxK	811.05	Joback Method
dvisc	0.0000993	Paxs	640.87	Joback Method
dvisc	0.0001341	Paxs	590.42	Joback Method

dvisc	0.0001915	Paxs	539.98	Joback Method
dvisc	0.0002942	Paxs	489.53	Joback Method
dvisc	0.0004990	Paxs	439.09	Joback Method
dvisc	0.0009707	Paxs	388.64	Joback Method
dvisc	0.0023029	Paxs	338.20	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R540920&Units=SI

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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