

3-Methoxybutyl caprylate

Inchi:	InChI=1S/C13H26O3/c1-4-5-6-7-8-9-13(14)16-11-10-12(2)15-3/h12H,4-11H2,1-3H3
InchiKey:	CSCXLFUSJVNPFR-UHFFFAOYSA-N
Formula:	C13H26O3
SMILES:	CCCCCCCC(=O)OCCC(C)OC
Mol. weight [g/mol]:	230.34

Physical Properties

Property code	Value	Unit	Source
gf	-282.78	kJ/mol	Joback Method
hf	-693.95	kJ/mol	Joback Method
hfus	29.88	kJ/mol	Joback Method
hvap	55.71	kJ/mol	Joback Method
log10ws	-3.33		Crippen Method
logp	3.315		Crippen Method
mvol	207.340	ml/mol	McGowan Method
pc	1694.90	kPa	Joback Method
rinpol	1526.00		NIST Webbook
rinpol	1526.00		NIST Webbook
tb	595.11	K	Joback Method
tc	766.49	K	Joback Method
tf	315.66	K	Joback Method
vc	0.799	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	543.85	J/molxK	595.11	Joback Method
cpg	619.34	J/molxK	737.93	Joback Method
cpg	605.53	J/molxK	709.37	Joback Method
cpg	591.08	J/molxK	680.80	Joback Method
cpg	575.99	J/molxK	652.24	Joback Method
cpg	560.25	J/molxK	623.67	Joback Method
cpg	632.50	J/molxK	766.49	Joback Method
dvisc	0.0001259	Paxs	595.11	Joback Method

dvisc	0.0001689	Paxs	548.54	Joback Method
dvisc	0.0002395	Paxs	501.96	Joback Method
dvisc	0.0003646	Paxs	455.38	Joback Method
dvisc	0.0006108	Paxs	408.81	Joback Method
dvisc	0.0011685	Paxs	362.23	Joback Method
dvisc	0.0027073	Paxs	315.66	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R540940&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log ₁₀ of Water solubility in mol/l
log_p:	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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