

3-Methoxybutyl heptanoate

Inchi:	InChI=1S/C12H24O3/c1-4-5-6-7-8-12(13)15-10-9-11(2)14-3/h11H,4-10H2,1-3H3
InchiKey:	LJFXZFKAYHQVRN-UHFFFAOYSA-N
Formula:	C12H24O3
SMILES:	CCCCCCC(=O)OCCC(C)OC
Mol. weight [g/mol]:	216.32

Physical Properties

Property code	Value	Unit	Source
gf	-291.20	kJ/mol	Joback Method
hf	-673.31	kJ/mol	Joback Method
hfus	27.29	kJ/mol	Joback Method
hvap	53.48	kJ/mol	Joback Method
log10ws	-2.91		Crippen Method
logp	2.925		Crippen Method
mcvol	193.250	ml/mol	McGowan Method
pc	1837.26	kPa	Joback Method
rinpol	1428.00		NIST Webbook
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tb	572.23	K	Joback Method
tc	744.65	K	Joback Method
tf	304.39	K	Joback Method
vc	0.744	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	492.37	J/molxK	572.23	Joback Method
cpg	508.15	J/molxK	600.97	Joback Method
cpg	523.31	J/molxK	629.70	Joback Method
cpg	537.87	J/molxK	658.44	Joback Method
cpg	551.82	J/molxK	687.18	Joback Method
cpg	565.17	J/molxK	715.92	Joback Method
cpg	577.91	J/molxK	744.65	Joback Method
dvisc	0.0029000	Paxs	304.39	Joback Method

dvisc	0.0012682	Paxs	349.03	Joback Method
dvisc	0.0006690	Paxs	393.67	Joback Method
dvisc	0.0004020	Paxs	438.31	Joback Method
dvisc	0.0002654	Paxs	482.95	Joback Method
dvisc	0.0001880	Paxs	527.59	Joback Method
dvisc	0.0001405	Paxs	572.23	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=R540960&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ 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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