

3-Methoxybutyl heptadecanoate

Inchi: InChI=1S/C22H44O3/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-22(23)25-20-19-21(2)2
InchiKey: JUBSFVZZAYGGLO-UHFFFAOYSA-N
Formula: C22H44O3
SMILES: CCCCCCCCCCCCCCCC(=O)OCCC(C)OC
Mol. weight [g/mol]: 356.58

Physical Properties

Property code	Value	Unit	Source
gf	-207.00	kJ/mol	Joback Method
hf	-879.71	kJ/mol	Joback Method
hfus	53.19	kJ/mol	Joback Method
hvap	75.74	kJ/mol	Joback Method
log10ws	-7.09		Crippen Method
logp	6.826		Crippen Method
mvol	334.150	ml/mol	McGowan Method
pc	922.18	kPa	Joback Method
rinpol	2422.00		NIST Webbook
rinpol	2422.00		NIST Webbook
tb	801.03	K	Joback Method
tc	981.83	K	Joback Method
tf	417.09	K	Joback Method
vc	1.304	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1065.16	J/molxK	801.03	Joback Method
cpg	1156.97	J/molxK	951.70	Joback Method
cpg	1140.73	J/molxK	921.57	Joback Method
cpg	1123.45	J/molxK	891.43	Joback Method
cpg	1105.11	J/molxK	861.30	Joback Method
cpg	1085.69	J/molxK	831.16	Joback Method
cpg	1172.19	J/molxK	981.83	Joback Method
dvisc	0.0000384	Paxs	801.03	Joback Method

dvisc	0.0000526	Paxs	737.04	Joback Method
dvisc	0.0000766	Paxs	673.05	Joback Method
dvisc	0.0001207	Paxs	609.06	Joback Method
dvisc	0.0002115	Paxs	545.07	Joback Method
dvisc	0.0004302	Paxs	481.08	Joback Method
dvisc	0.0010883	Paxs	417.09	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=R540955&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
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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