1-Methyl-2-methoxyethyl heneicosanoate

Inchi: InChI=1S/C25H50O3/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-25(26)28
InchiKey: YKFVOYHLOSXGTM-UHFFFAOYSA-N
Formula: C25H50O3
SMILES: CCCCCCCCCCCCCCCCCCCCC(=O)OC(C)COC
Mol. weight [g/mol]: 398.66

Physical Properties

Property code	Value	Unit	Source
gf	-181.74	kJ/mol	Joback Method
hf	-941.63	kJ/mol	Joback Method
hfus	60.96	kJ/mol	Joback Method
hvap	82.42	kJ/mol	Joback Method
log10ws	-8.35		Crippen Method
logp	7.996		Crippen Method
mcvol	376.420	ml/mol	McGowan Method
pc	779.81	kPa	Joback Method
rinpol	2700.00		NIST Webbook
tb	869.67	K	Joback Method
tc	1065.59	K	Joback Method
tf	450.90	K	Joback Method
vc	1.472	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1255.49	J/mol×K	869.67	Joback Method
cpg	1277.60	J/mol×K	902.32	Joback Method
cpg	1298.34	J/mol×K	934.98	Joback Method
cpg	1317.73	J/mol×K	967.63	Joback Method
cpg	1335.81	J/mol×K	1000.28	Joback Method
cpg	1352.62	J/mol×K	1032.94	Joback Method
cpg	1368.19	J/mol×K	1065.59	Joback Method
dvisc	0.0007426	Pa×s	450.90	Joback Method
dvisc	0.0002875	Pa×s	520.69	Joback Method

dvisc	0.0001393	Pa×s	590.49	Joback Method
dvisc	0.0000786	Pa×s	660.28	Joback Method
dvisc	0.0000495	Pa×s	730.08	Joback Method
dvisc	0.0000338	Pa×s	799.88	Joback Method
dvisc	0.0000246	Pa×s	869.67	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R540128&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