

Methyl 10,12-pentacosadiynoate

Inchi:	InChI=1S/C26H44O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25
InchiKey:	GGSURCIXQQGITI-UHFFFAOYSA-N
Formula:	C26H44O2
SMILES:	CCCCCCCCCCCC#CC#CCCCCCCCC(=O)OC
Mol. weight [g/mol]:	388.63
CAS:	120650-77-3

Physical Properties

Property code	Value	Unit	Source
gf	339.72	kJ/mol	Joback Method
hf	-280.17	kJ/mol	Joback Method
hfus	72.13	kJ/mol	Joback Method
hvap	86.93	kJ/mol	Joback Method
log10ws	-9.16		Crippen Method
logp	7.598		Crippen Method
mcvol	367.440	ml/mol	McGowan Method
pc	892.13	kPa	Joback Method
tb	888.57	K	Joback Method
tc	1089.26	K	Joback Method
tf	667.14	K	Joback Method
vc	1.440	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1183.03	J/molxK	888.57	Joback Method
cpg	1203.32	J/molxK	922.02	Joback Method
cpg	1222.39	J/molxK	955.47	Joback Method
cpg	1240.29	J/molxK	988.91	Joback Method
cpg	1257.05	J/molxK	1022.36	Joback Method
cpg	1272.73	J/molxK	1055.81	Joback Method
cpg	1287.36	J/molxK	1089.26	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C120650773&Units=SI
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

Legend

cpg:	Ideal gas heat capacity
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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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