13-Pentacosanone

Other names: pentacosan-13-one
Inchi: InChI=1S/C25H50O/c1-3-5-7-9-11-13-15-17-19-21-23-25(26)24-22-20-18-16-14-12-10-8
InchiKey: VTPOKROHHTWTML-UHFFFAOYSA-N
Formula: C25H50O
SMILES: CCCCCCCCCCCCC(=O)CCCCCCCCCCCC
Mol. weight [g/mol]: 366.66
CAS: 2123-19-5

Physical Properties

Property code	Value	Unit	Source
gf	30.70	kJ/mol	Joback Method
hf	-671.91	kJ/mol	Joback Method
hfus	62.10	kJ/mol	Joback Method
hvap	77.99	kJ/mol	Joback Method
log10ws	-9.57		Crippen Method
logp	9.178		Crippen Method
mcvol	364.680	ml/mol	McGowan Method
pc	791.26	kPa	Joback Method
tb	825.27	K	Joback Method
tc	1010.36	K	Joback Method
tf	421.44	K	Joback Method
vc	1.442	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1186.13	J/mol×K	825.27	Joback Method
cpg	1208.45	J/mol×K	856.12	Joback Method
cpg	1229.62	J/mol×K	886.97	Joback Method
cpg	1249.68	J/mol×K	917.82	Joback Method
cpg	1268.69	J/mol×K	948.66	Joback Method
cpg	1286.70	J/mol×K	979.51	Joback Method
cpg	1303.74	J/mol×K	1010.36	Joback Method
dvisc	0.0014199	Pa×s	421.44	Joback Method

dvisc	0.0005486	Pa×s	488.75	Joback Method
dvisc	0.0002668	Pa×s	556.05	Joback Method
dvisc	0.0001516	Pa×s	623.36	Joback Method
dvisc	0.0000962	Pa×s	690.66	Joback Method
dvisc	0.0000662	Pa×s	757.96	Joback Method
dvisc	0.0000484	Pa×s	825.27	Joback Method
hfust	96.17	kJ/mol	347.00	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2123195&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
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hfust: Enthalpy of fusion at a given temperature
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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume