(2E,6E,10E)-3,7,11,15-Tetramethylhexadeca-2,6,10 formate

Inchi: InChI=1S/C21H34O2/c1-18(2)9-6-10-19(3)11-7-12-20(4)13-8-14-21(5)15-16-23-17-22/h9
InchiKey: YCTKONHGXCYDJD-YKBIRWAZSA-N
Formula: C21H34O2
SMILES: CC(C)=CCCC(C)=CCCC(C)=CCCC(C)=CCOC=O
Mol. weight [g/mol]: 318.49
CAS: 125456-63-5

Physical Properties

Property code	Value	Unit	Source
gf	208.10	kJ/mol	Joback Method
hf	-264.85	kJ/mol	Joback Method
hfus	49.19	kJ/mol	Joback Method
hvap	71.62	kJ/mol	Joback Method
log10ws	-6.89		Crippen Method
logp	6.305		Crippen Method
mcvol	296.990	ml/mol	McGowan Method
pc	1149.87	kPa	Joback Method
rinpol	2233.60		NIST Webbook
rinpol	2233.60		NIST Webbook
tb	767.12	K	Joback Method
tc	957.97	K	Joback Method
tf	314.50	K	Joback Method
vc	1.171	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	871.04	J/mol×K	767.12	Joback Method
cpg	889.48	J/mol×K	798.93	Joback Method
cpg	907.05	J/mol×K	830.74	Joback Method
cpg	923.80	J/mol×K	862.54	Joback Method
cpg	939.81	J/mol×K	894.35	Joback Method
cpg	955.15	J/mol×K	926.16	Joback Method
cpg	969.90	J/mol×K	957.97	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C125456635&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
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