(E)-2-Hexyldec-2-enal

Inchi: InChI=1S/C16H30O/c1-3-5-7-9-10-12-14-16(15-17)13-11-8-6-4-2/h14-15H,3-13H2,1-2H3
InchiKey: RSBRHLFCWKXUSQ-JQIJEIRASA-N
Formula: C16H30O
SMILES: CCCCCCCC=C(C=O)CCCCCC
Mol. weight [g/mol]: 238.41

Physical Properties

Property code	Value	Unit	Source
gf	55.99	kJ/mol	Joback Method
hf	-351.72	kJ/mol	Joback Method
hfus	38.38	kJ/mol	Joback Method
hvap	57.97	kJ/mol	Joback Method
log10ws	-5.65		Crippen Method
logp	5.443		Crippen Method
mcvol	233.570	ml/mol	McGowan Method
pc	1453.46	kPa	Joback Method
rinpol	1769.00		NIST Webbook
ripol	2101.00		NIST Webbook
ripol	2101.00		NIST Webbook
tb	618.18	K	Joback Method
tc	789.51	K	Joback Method
tf	293.04	K	Joback Method
vc	0.929	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	624.12	J/mol×K	618.18	Joback Method
cpg	641.80	J/mol×K	646.74	Joback Method
cpg	658.68	J/mol×K	675.29	Joback Method
cpg	674.80	J/mol×K	703.85	Joback Method
cpg	690.18	J/mol×K	732.40	Joback Method
cpg	704.87	J/mol×K	760.96	Joback Method
cpg	718.89	J/mol×K	789.51	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R341901&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume