5-Dodecyl-5-ethylthiophene

Inchi: InChI=1S/C18H36S/c1-3-5-6-7-8-9-10-11-12-13-14-18-16-15-17(4-2)19-18/h17-18H,3-16
InchiKey: JQTLDXPHHFIIEM-UHFFFAOYSA-N
Formula: C18H36S
SMILES: CCCCCCCCCCCCC1CCC(CC)S1
Mol. weight [g/mol]: 284.54

Physical Properties

Property code	Value	Unit	Source
gf	169.38	kJ/mol	Joback Method
hf	-329.45	kJ/mol	Joback Method
hfus	41.04	kJ/mol	Joback Method
hvap	61.42	kJ/mol	Joback Method
log10ws	-7.36		Crippen Method
logp	6.972		Crippen Method
mcvol	269.970	ml/mol	McGowan Method
pc	1270.97	kPa	Joback Method
rinpol	2048.00		NIST Webbook
rinpol	2048.00		NIST Webbook
tb	669.68	K	Joback Method
tc	854.21	K	Joback Method
tf	382.73	K	Joback Method
vc	1.030	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	779.49	J/mol×K	669.68	Joback Method
cpg	801.45	J/mol×K	700.44	Joback Method
cpg	822.33	J/mol×K	731.19	Joback Method
cpg	842.16	J/mol×K	761.95	Joback Method
cpg	860.97	J/mol×K	792.70	Joback Method
cpg	878.80	J/mol×K	823.46	Joback Method
cpg	895.70	J/mol×K	854.21	Joback Method

Sources

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=R163969&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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