

9H-Fluorene-9-carboxylic acid, octadecyl ester

Inchi: InChI=1S/C32H46O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-21-26-34-32(33)31-29-24
InchiKey: MZYGBBQFBONXOA-UHFFFAOYSA-N
Formula: C32H46O2
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)C1c2ccccc2-c2ccccc21
Mol. weight [g/mol]: 462.71

Physical Properties

Property code	Value	Unit	Source
gf	275.15	kJ/mol	Joback Method
hf	-413.37	kJ/mol	Joback Method
hfus	71.06	kJ/mol	Joback Method
hvap	101.43	kJ/mol	Joback Method
log10ws	-11.20		Crippen Method
logp	9.604		Crippen Method
mcvol	410.800	ml/mol	McGowan Method
pc	801.60	kPa	Joback Method
rinpol	2507.00		NIST Webbook
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tb	1069.37	K	Joback Method
tc	1312.14	K	Joback Method
tf	625.42	K	Joback Method
vc	1.609	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1449.60	J/molxK	1069.37	Joback Method
cpg	1547.82	J/molxK	1271.68	Joback Method
cpg	1529.25	J/molxK	1231.22	Joback Method
cpg	1510.33	J/molxK	1190.75	Joback Method
cpg	1490.87	J/molxK	1150.29	Joback Method
cpg	1470.69	J/molxK	1109.83	Joback Method
cpg	1566.22	J/molxK	1312.14	Joback Method
dvisc	0.0001137	Paxs	1069.37	Joback Method

dvisc	0.0001373	Paxs	995.38	Joback Method
dvisc	0.0001708	Paxs	921.39	Joback Method
dvisc	0.0002209	Paxs	847.39	Joback Method
dvisc	0.0003001	Paxs	773.40	Joback Method
dvisc	0.0004350	Paxs	699.41	Joback Method
dvisc	0.0006884	Paxs	625.42	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=U415138&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log10 of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
p_c:	Critical Pressure
rin_{pol}:	Non-polar retention indices
t_b:	Normal Boiling Point Temperature
t_c:	Critical Temperature
t_f:	Normal melting (fusion) point
v_c:	Critical Volume

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