

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

Inchi: InChI=1S/C27H36O2/c1-2-3-4-5-6-7-8-9-10-11-16-21-29-27(28)26-24-19-14-12-17-22(23)13-20
InchiKey: PBSHVWRIKCGEJA-UHFFFAOYSA-N
Formula: C27H36O2
SMILES: CCCCCCCCCCOC(=O)C1c2ccccc2-c2ccccc21
Mol. weight [g/mol]: 392.57

Physical Properties

Property code	Value	Unit	Source
gf	233.05	kJ/mol	Joback Method
hf	-310.17	kJ/mol	Joback Method
hfus	58.11	kJ/mol	Joback Method
hvap	90.30	kJ/mol	Joback Method
log10ws	-9.11		Crippen Method
logp	7.653		Crippen Method
mcvol	340.350	ml/mol	McGowan Method
pc	1073.57	kPa	Joback Method
rinpol	3639.00		NIST Webbook
tb	954.97	K	Joback Method
tc	1173.00	K	Joback Method
tf	569.07	K	Joback Method
vc	1.329	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1130.64	J/molxK	954.97	Joback Method
cpg	1148.68	J/molxK	991.31	Joback Method
cpg	1165.80	J/molxK	1027.65	Joback Method
cpg	1182.12	J/molxK	1063.99	Joback Method
cpg	1197.76	J/molxK	1100.33	Joback Method
cpg	1212.84	J/molxK	1136.67	Joback Method
cpg	1227.46	J/molxK	1173.00	Joback Method
dvisc	0.0010614	Paxs	569.07	Joback Method
dvisc	0.0007114	Paxs	633.39	Joback Method

dvisc	0.0005133	Paxs	697.70	Joback Method
dvisc	0.0003913	Paxs	762.02	Joback Method
dvisc	0.0003112	Paxs	826.34	Joback Method
dvisc	0.0002558	Paxs	890.65	Joback Method
dvisc	0.0002159	Paxs	954.97	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=U415133&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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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