

2-Decyl nitrate

Inchi:	InChI=1S/C10H21NO3/c1-3-4-5-6-7-8-9-10(2)14-11(12)13/h10H,3-9H2,1-2H3
InchiKey:	OVYUFKGBDVSJT-UHFFFAOYSA-N
Formula:	C10H21NO3
SMILES:	CCCCCCCCC(C)O[N+](=O)[O-]
Mol. weight [g/mol]:	203.28

Physical Properties

Property code	Value	Unit	Source
gf	-38.57	kJ/mol	Joback Method
hf	-397.99	kJ/mol	Joback Method
hfus	30.68	kJ/mol	Joback Method
hvap	56.47	kJ/mol	Joback Method
log10ws	-4.28		Crippen Method
logp	3.334		Crippen Method
mcvol	175.050	ml/mol	McGowan Method
pc	2113.89	kPa	Joback Method
rmpol	1352.00		NIST Webbook
tb	602.02	K	Joback Method
tc	795.55	K	Joback Method
tf	353.30	K	Joback Method
vc	0.690	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	460.55	J/mol×K	602.02	Joback Method
cpg	475.78	J/mol×K	634.28	Joback Method
cpg	490.27	J/mol×K	666.53	Joback Method
cpg	504.04	J/mol×K	698.79	Joback Method
cpg	517.10	J/mol×K	731.04	Joback Method
cpg	529.48	J/mol×K	763.30	Joback Method
cpg	541.17	J/mol×K	795.55	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R496734&Units=SI

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
mccvol:	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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