

dodecyl 3,5-dinitrobenzoate

Inchi: InChI=1S/C19H28N2O6/c1-2-3-4-5-6-7-8-9-10-11-12-27-19(22)16-13-17(20(23)24)15-18
InchiKey: RNGZYLDMRQLQAR-UHFFFAOYSA-N
Formula: C19H28N2O6
SMILES: CCCCCCCCCCOC(=O)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1
Mol. weight [g/mol]: 380.44

Physical Properties

Property code	Value	Unit	Source
gf	39.43	kJ/mol	Joback Method
hf	-488.22	kJ/mol	Joback Method
hfus	63.74	kJ/mol	Joback Method
hvap	103.83	kJ/mol	Joback Method
log10ws	-7.62		Crippen Method
logp	5.581		Crippen Method
mcvol	297.090	ml/mol	McGowan Method
pc	1401.69	kPa	Joback Method
rinpol	2791.00		NIST Webbook
rinpol	2777.00		NIST Webbook
rinpol	2764.00		NIST Webbook
rinpol	2750.00		NIST Webbook
rinpol	2791.00		NIST Webbook
ripol	3719.00		NIST Webbook
ripol	3708.00		NIST Webbook
ripol	3690.00		NIST Webbook
tb	1050.73	K	Joback Method
tc	1290.47	K	Joback Method
tf	714.73	K	Joback Method
vc	1.179	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	991.56	J/molxK	1050.73	Joback Method
cpg	1003.17	J/molxK	1090.69	Joback Method

cpg	1013.54	J/mol×K	1130.64	Joback Method
cpg	1022.72	J/mol×K	1170.60	Joback Method
cpg	1030.79	J/mol×K	1210.55	Joback Method
cpg	1037.80	J/mol×K	1250.51	Joback Method
cpg	1043.82	J/mol×K	1290.47	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R312379&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
rinpola:	Non-polar retention indices
ripola:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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