

Hexyl 3,4-dimethylbenzoate

Inchi:	InChI=1S/C15H22O2/c1-4-5-6-7-10-17-15(16)14-9-8-12(2)13(3)11-14/h8-9,11H,4-7,10H
InchiKey:	NUPRBGNIFNXSFI-UHFFFAOYSA-N
Formula:	C15H22O2
SMILES:	CCCCCCOC(=O)c1ccc(C)c(C)c1
Mol. weight [g/mol]:	234.33

Physical Properties

Property code	Value	Unit	Source
gf	-65.35	kJ/mol	Joback Method
hf	-384.14	kJ/mol	Joback Method
hfus	30.66	kJ/mol	Joback Method
hvap	61.74	kJ/mol	Joback Method
log10ws	-4.76		Crippen Method
logp	4.041		Crippen Method
mcvol	205.890	ml/mol	McGowan Method
pc	1872.41	kPa	Joback Method
rinsol	1645.00		NIST Webbook
tb	655.53	K	Joback Method
tc	854.78	K	Joback Method
tf	382.43	K	Joback Method
vc	0.791	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	545.77	J/molxK	655.53	Joback Method
cpg	562.20	J/molxK	688.74	Joback Method
cpg	577.76	J/molxK	721.95	Joback Method
cpg	592.46	J/molxK	755.16	Joback Method
cpg	606.32	J/molxK	788.36	Joback Method
cpg	619.37	J/molxK	821.57	Joback Method
cpg	631.60	J/molxK	854.78	Joback Method
dvisc	0.0012115	Paxs	382.43	Joback Method
dvisc	0.0006904	Paxs	427.95	Joback Method

dvisc	0.0004383	Paxs	473.46	Joback Method
dvisc	0.0003014	Paxs	518.98	Joback Method
dvisc	0.0002201	Paxs	564.50	Joback Method
dvisc	0.0001685	Paxs	610.01	Joback Method
dvisc	0.0001339	Paxs	655.53	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=R543221&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
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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