

hexyl-d3 hexanoate-d3

Inchi:	InChI=1S/C12H24O2/c1-3-5-7-9-11-14-12(13)10-8-6-4-2/h3-11H2,1-2H3/i1D3,2D3
InchiKey:	NCDCLPBOMHPFCV-WFGJKAKNSA-N
Formula:	C12H18D6O2
SMILES:	CCCCCOC(=O)CCCCC
Mol. weight [g/mol]:	206.35

Physical Properties

Property code	Value	Unit	Source
gf	-183.76	kJ/mol	Joback Method
hf	-535.81	kJ/mol	Joback Method
hfus	29.62	kJ/mol	Joback Method
hvap	51.46	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	3.690		Crippen Method
mcvol	187.380	ml/mol	McGowan Method
pc	1851.52	kPa	Joback Method
ripol	1601.00		NIST Webbook
tb	550.25	K	Joback Method
tc	720.05	K	Joback Method
tf	297.16	K	Joback Method
vc	0.732	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	464.17	J/molxK	550.25	Joback Method
cpg	479.84	J/molxK	578.55	Joback Method
cpg	494.90	J/molxK	606.85	Joback Method
cpg	509.36	J/molxK	635.15	Joback Method
cpg	523.23	J/molxK	663.45	Joback Method
cpg	536.51	J/molxK	691.75	Joback Method
cpg	549.22	J/molxK	720.05	Joback Method
dvisc	0.0030867	Paxs	297.16	Joback Method
dvisc	0.0014485	Paxs	339.34	Joback Method

dvisc	0.0008035	Paxs	381.52	Joback Method
dvisc	0.0005012	Paxs	423.70	Joback Method
dvisc	0.0003406	Paxs	465.89	Joback Method
dvisc	0.0002467	Paxs	508.07	Joback Method
dvisc	0.0001878	Paxs	550.25	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R329085&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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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