

hexyl 2-methylbutanoate-d-3

Inchi:	InChI=1S/C11H22O2/c1-4-6-7-8-9-13-11(12)10(3)5-2/h10H,4-9H2,1-3H3/i2D3
InchiKey:	YUECNVSODFDKOQ-BMSJAHLVSA-N
Formula:	C11H19D3O2
SMILES:	CCCCCOC(=O)C(C)CC
Mol. weight [g/mol]:	189.31

Physical Properties

Property code	Value	Unit	Source
gf	-194.62	kJ/mol	Joback Method
hf	-520.45	kJ/mol	Joback Method
hfus	23.51	kJ/mol	Joback Method
hvap	48.85	kJ/mol	Joback Method
log10ws	-3.05		Crippen Method
logp	3.156		Crippen Method
mcvol	173.290	ml/mol	McGowan Method
pc	2029.06	kPa	Joback Method
ripol	1423.00		NIST Webbook
tb	526.93	K	Joback Method
tc	701.19	K	Joback Method
tf	270.89	K	Joback Method
vc	0.669	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	415.48	J/molxK	526.93	Joback Method
cpg	430.78	J/molxK	555.97	Joback Method
cpg	445.49	J/molxK	585.02	Joback Method
cpg	459.60	J/molxK	614.06	Joback Method
cpg	473.13	J/molxK	643.11	Joback Method
cpg	486.09	J/molxK	672.15	Joback Method
cpg	498.48	J/molxK	701.19	Joback Method
dvisc	0.0044896	Paxs	270.89	Joback Method
dvisc	0.0018616	Paxs	313.56	Joback Method

dvisc	0.0009531	Paxs	356.24	Joback Method
dvisc	0.0005632	Paxs	398.91	Joback Method
dvisc	0.0003684	Paxs	441.58	Joback Method
dvisc	0.0002597	Paxs	484.26	Joback Method
dvisc	0.0001937	Paxs	526.93	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R322702&Units=SI

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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