

2-methylbutyl-d-3 2-methylbutanoate

Inchi:	InChI=1S/C10H20O2/c1-5-8(3)7-12-10(11)9(4)6-2/h8-9H,5-7H2,1-4H3/i1D3
InchiKey:	PVYFCGRBIREQLL-FIBGUPNXSA-N
Formula:	C10H17D3O2
SMILES:	CCC(C)COC(=O)C(C)CC
Mol. weight [g/mol]:	175.28

Physical Properties

Property code	Value	Unit	Source
gf	-205.48	kJ/mol	Joback Method
hf	-505.09	kJ/mol	Joback Method
hfus	17.40	kJ/mol	Joback Method
hvap	46.23	kJ/mol	Joback Method
log10ws	-2.39		Crippen Method
logp	2.622		Crippen Method
mcvol	159.200	ml/mol	McGowan Method
pc	2233.41	kPa	Joback Method
ripol	1283.00		NIST Webbook
tb	503.61	K	Joback Method
tc	682.96	K	Joback Method
tf	244.62	K	Joback Method
vc	0.608	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	368.51	J/molxK	503.61	Joback Method
cpg	437.08	J/molxK	653.07	Joback Method
cpg	424.51	J/molxK	623.18	Joback Method
cpg	411.38	J/molxK	593.28	Joback Method
cpg	397.67	J/molxK	563.39	Joback Method
cpg	383.39	J/molxK	533.50	Joback Method
cpg	449.08	J/molxK	682.96	Joback Method
dvisc	0.0001994	Paxs	503.61	Joback Method
dvisc	0.0002734	Paxs	460.44	Joback Method

dvisc	0.0004002	Paxs	417.28	Joback Method
dvisc	0.0006396	Paxs	374.12	Joback Method
dvisc	0.0011553	Paxs	330.95	Joback Method
dvisc	0.0024917	Paxs	287.79	Joback Method
dvisc	0.0070487	Paxs	244.62	Joback Method

Sources

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=R322544&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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