

2-methylbutyl-d-3 heptanoate

Inchi:	InChI=1S/C12H24O2/c1-4-6-7-8-9-12(13)14-10-11(3)5-2/h11H,4-10H2,1-3H3/i2D3
InchiKey:	NEYFHTHRJVQMPA-BMSJAHLVSA-N
Formula:	C12H21D3O2
SMILES:	CCCCCCC(=O)OCC(C)CC
Mol. weight [g/mol]:	203.34

Physical Properties

Property code	Value	Unit	Source
gf	-186.20	kJ/mol	Joback Method
hf	-541.09	kJ/mol	Joback Method
hfus	26.10	kJ/mol	Joback Method
hvap	51.07	kJ/mol	Joback Method
log10ws	-3.47		Crippen Method
logp	3.546		Crippen Method
mcvol	187.380	ml/mol	McGowan Method
pc	1864.33	kPa	Joback Method
ripol	1554.00		NIST Webbook
ripol	1554.00		NIST Webbook
tb	549.81	K	Joback Method
tc	722.69	K	Joback Method
tf	282.16	K	Joback Method
vc	0.726	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	464.44	J/molxK	549.81	Joback Method
cpg	480.46	J/molxK	578.62	Joback Method
cpg	495.83	J/molxK	607.44	Joback Method
cpg	510.57	J/molxK	636.25	Joback Method
cpg	524.69	J/molxK	665.07	Joback Method
cpg	538.20	J/molxK	693.88	Joback Method
cpg	551.11	J/molxK	722.69	Joback Method
dvisc	0.0042661	Paxs	282.16	Joback Method

dvisc	0.0017460	Paxs	326.77	Joback Method
dvisc	0.0008857	Paxs	371.38	Joback Method
dvisc	0.0005197	Paxs	415.99	Joback Method
dvisc	0.0003381	Paxs	460.59	Joback Method
dvisc	0.0002373	Paxs	505.20	Joback Method
dvisc	0.0001764	Paxs	549.81	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R322584&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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