

2-methylbutyl-d-3 octanoate

Inchi:	InChI=1S/C13H26O2/c1-4-6-7-8-9-10-13(14)15-11-12(3)5-2/h12H,4-11H2,1-3H3/i2D3
InchiKey:	XZLBJDGPiWDVIJ-BMSJAHLVSA-N
Formula:	C13H23D3O2
SMILES:	CCCCCCCC(=O)OCC(C)CC
Mol. weight [g/mol]:	217.36

Physical Properties

Property code	Value	Unit	Source
gf	-177.78	kJ/mol	Joback Method
hf	-561.73	kJ/mol	Joback Method
hfus	28.69	kJ/mol	Joback Method
hvap	53.30	kJ/mol	Joback Method
log10ws	-3.88		Crippen Method
logp	3.936		Crippen Method
mvol	201.470	ml/mol	McGowan Method
pc	1718.88	kPa	Joback Method
ripol	1655.00		NIST Webbook
ripol	1655.00		NIST Webbook
tb	572.69	K	Joback Method
tc	744.36	K	Joback Method
tf	293.43	K	Joback Method
vc	0.781	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	515.10	J/molxK	572.69	Joback Method
cpg	531.74	J/molxK	601.30	Joback Method
cpg	547.70	J/molxK	629.91	Joback Method
cpg	563.00	J/molxK	658.53	Joback Method
cpg	577.64	J/molxK	687.14	Joback Method
cpg	591.64	J/molxK	715.75	Joback Method
cpg	605.00	J/molxK	744.36	Joback Method
dvisc	0.0040106	Paxs	293.43	Joback Method

dvisc	0.0016218	Paxs	339.97	Joback Method
dvisc	0.0008156	Paxs	386.52	Joback Method
dvisc	0.0004755	Paxs	433.06	Joback Method
dvisc	0.0003078	Paxs	479.60	Joback Method
dvisc	0.0002152	Paxs	526.15	Joback Method
dvisc	0.0001594	Paxs	572.69	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R322608&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

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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