

butyl heptanoate-d13

Inchi:	InChI=1S/C11H22O2/c1-3-5-7-8-9-11(12)13-10-6-4-2/h3-10H2,1-2H3/i1D3,3D2,5D2,7D2
InchiKey:	YPQSPODHFVAC-DMMZKVCBSA-N
Formula:	C11H9D13O2
SMILES:	CCCCCCC(=O)OCCCC
Mol. weight [g/mol]:	199.37

Physical Properties

Property code	Value	Unit	Source
gf	-192.18	kJ/mol	Joback Method
hf	-515.17	kJ/mol	Joback Method
hfus	27.03	kJ/mol	Joback Method
hvap	49.24	kJ/mol	Joback Method
log10ws	-3.29		Crippen Method
logp	3.300		Crippen Method
mvol	173.290	ml/mol	McGowan Method
pc	2014.51	kPa	Joback Method
ripol	1498.00		NIST Webbook
tb	527.37	K	Joback Method
tc	698.36	K	Joback Method
tf	285.89	K	Joback Method
vc	0.675	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	415.24	J/molxK	527.37	Joback Method
cpg	430.19	J/molxK	555.87	Joback Method
cpg	444.58	J/molxK	584.37	Joback Method
cpg	458.41	J/molxK	612.87	Joback Method
cpg	471.67	J/molxK	641.36	Joback Method
cpg	484.39	J/molxK	669.86	Joback Method
cpg	496.57	J/molxK	698.36	Joback Method
dvisc	0.0032030	Paxs	285.89	Joback Method
dvisc	0.0015281	Paxs	326.14	Joback Method

dvisc	0.0008577	Paxs	366.38	Joback Method
dvisc	0.0005398	Paxs	406.63	Joback Method
dvisc	0.0003692	Paxs	446.88	Joback Method
dvisc	0.0002689	Paxs	487.12	Joback Method
dvisc	0.0002056	Paxs	527.37	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R328928&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

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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