

6-Methylhept-4-en-1-yl isobutyrate

Inchi:	InChI=1S/C12H22O2/c1-10(2)8-6-5-7-9-14-12(13)11(3)4/h6,8,10-11H,5,7,9H2,1-4H3/b8-
InchiKey:	JDRFSFLYVBOTAT-SOFGYWHQSA-N
Formula:	C12H22O2
SMILES:	CC(C)C=CCCCOC(=O)C(C)C
Mol. weight [g/mol]:	198.30
CAS:	1215128-03-2

Physical Properties

Property code	Value	Unit	Source
gf	-108.42	kJ/mol	Joback Method
hf	-429.15	kJ/mol	Joback Method
hfus	22.78	kJ/mol	Joback Method
hvap	50.64	kJ/mol	Joback Method
log10ws	-3.08		Crippen Method
logp	3.178		Crippen Method
mcvol	183.080	ml/mol	McGowan Method
pc	1964.82	kPa	Joback Method
rinpol	1293.20		NIST Webbook
rinpol	1293.20		NIST Webbook
tb	553.53	K	Joback Method
tc	736.79	K	Joback Method
tf	262.08	K	Joback Method
vc	0.700	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	446.33	J/molxK	553.53	Joback Method
cpg	462.35	J/molxK	584.07	Joback Method
cpg	477.65	J/molxK	614.62	Joback Method
cpg	492.24	J/molxK	645.16	Joback Method
cpg	506.15	J/molxK	675.70	Joback Method
cpg	519.39	J/molxK	706.25	Joback Method
cpg	531.97	J/molxK	736.79	Joback Method

dvisc	0.0059039	Paxs	262.08	Joback Method
dvisc	0.0019456	Paxs	310.66	Joback Method
dvisc	0.0008657	Paxs	359.23	Joback Method
dvisc	0.0004671	Paxs	407.81	Joback Method
dvisc	0.0002874	Paxs	456.38	Joback Method
dvisc	0.0001942	Paxs	504.95	Joback Method
dvisc	0.0001405	Paxs	553.53	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1215128032&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
mvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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