

butyl 2,4-dimethylheptanoate

Inchi:	InChI=1S/C13H26O2/c1-5-7-9-15-13(14)12(4)10-11(3)8-6-2/h11-12H,5-10H2,1-4H3
InchiKey:	VTQXILGYVYSPGZ-UHFFFAOYSA-N
Formula:	C13H26O2
SMILES:	CCCCOC(=O)C(C)CC(C)CCC
Mol. weight [g/mol]:	214.34

Physical Properties

Property code	Value	Unit	Source
gf	-180.22	kJ/mol	Joback Method
hf	-567.01	kJ/mol	Joback Method
hfus	25.17	kJ/mol	Joback Method
hvap	52.91	kJ/mol	Joback Method
log10ws	-3.64		Crippen Method
logp	3.792		Crippen Method
mcvol	201.470	ml/mol	McGowan Method
pc	1730.34	kPa	Joback Method
ripol	1549.00		NIST Webbook
ripol	1549.00		NIST Webbook
tb	572.25	K	Joback Method
tc	746.93	K	Joback Method
tf	278.43	K	Joback Method
vc	0.775	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	515.40	J/molxK	572.25	Joback Method
cpg	532.39	J/molxK	601.36	Joback Method
cpg	548.66	J/molxK	630.48	Joback Method
cpg	564.24	J/molxK	659.59	Joback Method
cpg	579.14	J/molxK	688.70	Joback Method
cpg	593.36	J/molxK	717.82	Joback Method
cpg	606.91	J/molxK	746.93	Joback Method
dvisc	0.0057377	Paxs	278.43	Joback Method

dvisc	0.0019823	Paxs	327.40	Joback Method
dvisc	0.0009030	Paxs	376.37	Joback Method
dvisc	0.0004930	Paxs	425.34	Joback Method
dvisc	0.0003050	Paxs	474.31	Joback Method
dvisc	0.0002064	Paxs	523.28	Joback Method
dvisc	0.0001494	Paxs	572.25	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R493235&Units=SI

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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