Diethylmalonic acid, 4-bromobenzyl heptyl ester

Inchi: InChI=1S/C21H31BrO4/c1-4-7-8-9-10-15-25-19(23)21(5-2,6-3)20(24)26-16-17-11-13-18(

InchiKey: KEUQDSIGZMYNFA-UHFFFAOYSA-N

Formula: C21H31BrO4

SMILES: CCCCCCCOC(=O)C(CC)(CC)C(=O)OCc1ccc(Br)cc1

Mol. weight [g/mol]: 427.37

Physical Properties

Property code	Value	Unit	Source
gf	-221.96	kJ/mol	Joback Method
hf	-723.73	kJ/mol	Joback Method
hfus	47.24	kJ/mol	Joback Method
hvap	88.73	kJ/mol	Joback Method
log10ws	-6.86		Crippen Method
logp	5.812		Crippen Method
mcvol	315.370	ml/mol	McGowan Method
pc	1333.93	kPa	Joback Method
rinpol	2558.00		NIST Webbook
rinpol	2558.00		NIST Webbook
tb	927.05	K	Joback Method
tc	1143.73	K	Joback Method
tf	571.91	K	Joback Method
vc	1.202	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	978.07	J/mol×K	927.05	Joback Method
cpg	992.85	J/mol×K	963.16	Joback Method
cpg	1006.49	J/mol×K	999.28	Joback Method
cpg	1019.04	J/mol×K	1035.39	Joback Method
cpg	1030.58	J/mol×K	1071.50	Joback Method
cpg	1041.16	J/mol×K	1107.62	Joback Method
cpg	1050.85	J/mol×K	1143.73	Joback Method
dvisc	0.0003024	Pa×s	571.91	Joback Method

dvisc	0.0001694	Pa×s	631.10	Joback Method
dvisc	0.0001049	Pa×s	690.29	Joback Method
dvisc	0.0000700	Pa×s	749.48	Joback Method
dvisc	0.0000496	Pa×s	808.67	Joback Method
dvisc	0.0000368	Pa×s	867.86	Joback Method
dvisc	0.0000284	Pa×s	927.05	Joback Method

Sources

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=U368451&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume