Diethylmalonic acid, 1-bromo-3,3,3-trifluoroprop-2-yl hexadecyl ester

Inchi: InChI=1S/C26H46BrF3O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-19-20-33-23(31)25(5-

InchiKey: KORFQBVYAWEYGL-UHFFFAOYSA-N

Formula: C26H46BrF3O4

SMILES: CCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OC(CBr)C(F)(F)F

Mol. weight [g/mol]: 559.54

Physical Properties

Property code	Value	Unit	Source
gf	-866.67	kJ/mol	Joback Method
hf	-1654.35	kJ/mol	Joback Method
hfus	64.84	kJ/mol	Joback Method
hvap	92.79	kJ/mol	Joback Method
log10ws	-9.40		Crippen Method
logp	8.686		Crippen Method
mcvol	414.890	ml/mol	McGowan Method
pc	753.91	kPa	Joback Method
rinpol	2735.00		NIST Webbook
rinpol	2735.00		NIST Webbook
tb	1003.93	K	Joback Method
tc	1240.32	K	Joback Method
tf	578.51	K	Joback Method
vc	1.627	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1411.52	J/mol×K	1003.93	Joback Method
cpg	1431.08	J/mol×K	1043.33	Joback Method
cpg	1449.22	J/mol×K	1082.73	Joback Method
cpg	1466.08	J/mol×K	1122.13	Joback Method
cpg	1481.78	J/mol×K	1161.53	Joback Method
cpg	1496.47	J/mol×K	1200.92	Joback Method
cpg	1510.27	J/mol×K	1240.32	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=U370808&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
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